Empowered corrosion-resistant products through HCP crystal network: a topological assistance

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ABSTRACT

Human computer interaction (HCI) aims to enhance product effectiveness and efficiency by empowering users. This research examines corrosion resistance in alloys, a concern due to technological advancements. Metals and alloys are susceptible to degradation, leading to functionality loss, structural collapse, and environmental contamination. Improving corrosion resistance is crucial for product efficiency. In this paper, HCI identifies requirements that emphasize taking an existing hexagonal closely packed (HCP) network, investigating the network for requirements in the form of vertices and edges, mapping different vertices and edges of the network graph with topological invariants, solving the network graph by invariants, and providing results for modeling and design of advanced networks and architectures. The HCI also ensures and investigates the optimization of results produced under the specifications. The study examines network graph results for irregularities, providing guidelines for engineers and manufacturers to create advanced alloy architectures with characteristics through mathematical and graphical methods.

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1. INTRODUCTION

Human computer interaction (HCI) is a science used to enhance the effectiveness, and efficiency of apps and products used by humans and deals with every aspect of products to empower them. This study deals with the crystal structures used in alloys and how they improve corrosion resistance. The hexagonal closed-packed (HCP) Crystal structure has three levels of atoms. Six atoms form a hexagonal arrangement in the top and bottom layers, while a seventh atom sits in the center of the hexagonal arrangement. Three atoms in the intermediate layer are tucked away in the top and bottom plane's triangular grooves. Alternating layers' hexagonal structures are altered so that their atoms line up with the gaps of the layer before them. Similar to the fcc structure, the atoms from one layer nestle among those of the adjacent layer in that area. The pattern, though, is hexagonal rather than cubic. The packing factor is equal to the fcc unit cell at 0.74. In a hexagonal close-packed configuration, the atoms effectively occupy 74% of the space, leaving 26% unoccupied. With a coordination number of 12, the hexagonal closest packing has six atoms per unit cell. Slip is significantly more constrained in HCP metals than in body-centered cubic and face-centered cubic crystal forms.

Normally, the densely packed basal planes of HCP crystal formations enable slide. Other slip planes' activation is influenced by several factors, including the c/a ratio. Since there are only three independent slip systems on the basal planes, extra slip or twin systems must be triggered for arbitrary plastic deformation. HCP polycrystals often exhibit brittle behavior as a result of this, which typically calls for significantly greater resolved shear stress. Cobalt and zinc are examples of HCP metals that are less ductile than fcc metals. Magnesium is an extremely brittle HCP metal, while titanium is a relatively ductile metal [1]. Today's society depends on metals and alloys for many of our daily tasks. The change of the metal or alloy to its more thermodynamically favored oxide or hydroxide phase, however, makes them susceptible to corrosion. These unfavorable corrosion reactions can cause metallic components to fail. As a result, corrosion-protective technologies are more crucial than ever because they are necessary to cut down on the waste of priceless resources. This review explores the role of layered and 2D materials, particularly transition metal dichalcogenides, in creating effective corrosion prevention strategies [2].

In today's civilization, metals and alloys are crucial, and depending on their characteristics, they have a wide range of uses. Aluminum and titanium, for instance, are both lightweight and used in the aerospace sector, while copper or copper that has been electroplated is frequently used in electrical applications and steel is used in building and transportation. Metals and alloys are susceptible to corrosion despite technological advancements in processing that have improved their performance. When a pure metal or alloy comes into touch with its environment, a natural process occurs that transforms it into the thermodynamically preferred oxide, hydroxide, carbonate, or sulphide. As a result, the material slowly degrades and disintegrates, which may eventually cause a loss of functionality, structural collapse, or even environmental contamination due to the discharge of potentially dangerous metal ions. To replace the failed component, additional metals or alloys are frequently used, which has an impact on sustainability due to the excessive use of natural resources. In the modern world, sustainability is a crucial factor to take into account. Innovative corrosion-protection techniques are thus needed to reduce the need for early metal and alloy repair or replacement. This paper discusses the use of k-banhatti sombor invariants, which have predictive properties for various variants of HCP graphs or networks, in various fields such as physics, computer science, mathematics, chemistry, pharmacy, informatics, and biology, despite their lack of reliable analysis. The study resolved the topology of HCP network graphs [3], [4].

After Gutman's Sombor indices in 2021, V. R. Kulli introduced various topological degree-based indices. Dharwad Indices are the name of these indices. It has a few other forms that are utilized to solve the topology of aromatic compounds, including reduced Dharwad, reduced Dharwad exponential, and the Dharwad index. These indices can be used to quickly and effectively solve the topology of a graph and determine the bottom and upper boundaries of networks or graphs. Another emerging field of study is cheminformatics, which combines chemistry, mathematics, and computer sciences. Its key components include quantitative structure-activity relationships (QSAR) and structure-property relationships (QSPR), which can add to the analysis of synthetic mixtures' physicochemical properties. A topological index is strongly associated with a graph that is invariant under graph automorphism and can depict the geography of a graph as a numeric number. In the underlying chemistry, graph theory has a variety of applications [5], [6].

The study has significance for modeling the purpose of networks, network connections, powergenerating interconnection networks, and chemical compounds in the domain of physics, chemistry, computer science, mathematics, and bioinformatics. We can learn more about algebraic structures and use mathematics to forecast their hidden characteristics, such as those of certain computer networks, thanks to the ISO and KBRZ invariants [7], [8]. This paper explores the use of contra harmonic-quadratic invariants (CQIs) in solving HCP networks, demonstrating their potential applications in various fields. Two types of CQI and quadratic-contra harmonic indices were used in the study to determine the geography of HCP graphs/networks. The determined results can be used to model the aforementioned networks [9].

The study solves the topology of the HCP network structure mathematically by graph theory. The study modeled the HCP network structure with the help of deduced mathematical results. The study enhanced the existing HCP network structure used for improved corrosion-resistant products, reduced their irregularities, and found side effect-free, stable products, and efficient alloys in the context of stability and corrosion resistance. The HCP network structure is mapped and solved by graph theory after converting it into graphical form, producing mathematical results for modeling the HCP network structures.

This research aims to optimize existing HCP network structures for stable and corrosion-resistive products by analyzing topological invariants and graphing HCP network structures. It will develop QSPR and QSAR models, discover the relationship between lower and upper bounds, and provide design guidelines for corrosion-resistive product developers. Due to the incremental and fast nature of population increase, more stable and corrosion-resistive products are required, but no adequate solution has been found till now. The study wants to find new efficient, stable, and corrosion-resistive network structures and products.

2. LITERATURE REVIEW

A more recent idea is the evaluation of degree-based topological indices using M-polynomials. The Hex-derived network, which derives from the hexagonal network, has a variety of uses in the fields of electronics, pharmaceuticals, and telecommunications networks. In the current study, we produce a three-dimensional, subdivided chain Hex-derived network. We use the direct technique and the M-polynomial method to determine the degree-dependent topological indices of the divided network. To comprehend the geometric behavior of the M-polynomial and the accompanying topological descriptors of the mentioned network, we also visually display them. The data obtained can serve as a foundation for further study of subdivided chain Hex-derived networks, their characteristics, and their uses [9].

In a network with a hexagonal topology, heuristic shortest path routing methods and performance evaluation are suggested for determining the best optical path between two optical switch nodes. The benefits of hexagonal optical switching networks are flexibility and fault tolerance. We can increase the level count to expand the hexagonal topology network. The routing algorithm and a 7-level hexagonal topology network with 294 nodes have both been built. The performance of a four-level hexagonal topology network was assessed using a variety of methods, including shortest path routing algorithm with artificial intelligence using decision trees (SPRA-AI), shortest path routing algorithm with spanning trees (SPRA-SPT), and shortest path routing algorithm with pure distance prediction (SPRA-PDP). For the simulation findings to be accurate, the simulated traffic mode is also recorded from the real core network [10].

A graph invariant is any integer that a graph can independently identify and change. This study explores three bridge networks: Sierpinski, honeycomb, and hexagonal networks, with the irregularity sombor invariant introduced for various network properties. Utilize the irregularity Sombor Index to first identify the irregularities in the networks. This will be done in a step-by-step fashion [11]. In the discipline of material sciences, honeycomb networks are particularly important for wireless base stations, image processing, and graphics. By repeatedly using hexagonal tiles in a specific pattern, honeycomb networks are created. We're referring to the n-layered, HCn-based honeycomb network with hexagons between the focal and boundary hexagons. HCn is created by enclosing HCn1 in a layer of hexagons. Other computer science areas like microprocessors, memory connections, and processor interconnection can benefit from its examination [12].

This work introduces a new methodology for estimating the functional vulnerability of Catania's road network using spatial-temporal mobility profiles from floating automobile data, contrasting the conventional topological data-based approach. The technique evaluates the impact of failure events on trajectories and travel times. Every time a road link is broken, the algorithm's basic operation is based on computing all potential travel routes inside the designated geographical zone. The process might help with evaluating large-scale failure situations and facilitating emergency plans [13].

This study optimizes a free-form hole shape for square and hexagonal lattice aluminum plate PnCs with high relative bandgaps using deep neural networks' predictive abilities. The initial training dataset consists of 20,000 randomly produced unit cells with symmetric smooth holes. Finite element analysis is used to assess relative bandgap, and genetic optimization techniques are used to find design candidates with large relative band gaps. Using FEA, the relative bandgaps of new candidates are identified and verified. Active learning is performed to update the DNNs using the analysis results. For square and hexagonal lattices, it is discovered that the iteratively optimized hole shapes have greater band gaps than circular holes [14].

A network lattice serves as the spatial substrate in our proposed minimum model for the formation of spatial networks, and edge velocities and distances define an effective temporal distance that measures the effectiveness of exploring urban space. To derive origin-destination matrices, we simulate these flows from the viewpoint of urban transportation using human mobility models. We discover that when utilizing basic lattices, the generated optimal topologies change depending on the spatial range of flows from tree-like structures to more regular networks. Surprisingly, when the network is tuned for the interaction between diverse mobility patterns of short-distance travels and longer-distance ones typical of commuting, we discover that branches paired to big loop structures appear as ideal architectures. Finally, we demonstrate that the statistical spatial features of the Greater London Area subway network can be recovered using our methodology [15].

As seen from the literature review, the honeycomb networks, hex-derived networks, and n-layered hexagonal networks are used in different fields to increase the resilience of urban transportation during critical events, increase the efficiency of wireless base stations, image processing, develop heuristic shortest path routing methods and performance evaluation. Uses in the fields of electronics, pharmaceuticals, telecommunications networks, effectively a modification of elastic waves, phononic crystals (PnCs) with a broad bandgap, and for the formation of spatial networks. In contrast, the study solved hexagonal closely-packed crystal structures for the improvements of alloys to enhance the corrosion resistivity by topological attempt.

3. PROPOSED METHOD

The approach is grounded in quantitative research in which HCI is involved. The goal of this study is to investigate and clarify important issues related to HCP structures like corrosion-free, effective use, and improved capabilities in products and chemical compounds which are the attributes of HCI. It provides modeling expression after mapping and solving the existing HCP network by topological invariants.

3.1. The method with integration of HCI

At first, HCI identifies requirements that emphasize taking an existing HCP network. Investigate the network for getting requirements in the form of vertices and edges of the network. In the mapping, phase found the suitable topological invariants for the mapping of the network graph. HCI's third phase covers the actual mapping of different vertices and edges of the network graph with topological invariants and in the design and experimentation phase, HCI solves the network graph by invariants and gives results for modeling and design of advanced networks and architectures. In the fourth phase Evaluation and Optimization against Requirements, the HCI ensures and investigates the optimization of the results produced in the previous phase according to the requirements [16]. In the fifth phase System Satisfaction, the HCI ensures that results satisfy the requirements if not then in the next phase, the HCI compels to check the irregularities from the results of the network graph and produces results of irregularities against the given network graph. After that, it may repeat the whole process till the optimized mathematical and graphical results are found with the best characteristics of the given network. The study will use KBSO, QCIs, KBRZs, Dharwad invariants, their reduced forms, and the ISO index to solve the network graph's topology. The formula-based determined results will be compared to previous findings and used to simulate particular items and chemical substances [17]-[23]. This model is highly disruptive by indulging HCI since it constructs an HCP network's geography using numbers and graphics and produces optimum outcomes. After the assessment, results are confirmed and endorsed using a tool called Maple [24], [25].

Figure 1 shows the orderly review, which will take an existing HCP network structure and associate it with a graph after finding the vertices and edges of that network and solve the topology of the graph with the assistance of k-banhatti Sombor lists, its decreased structure, QCI, the CQI, the Dharwad index, its diminished structure, and three different types of KBRZ files. The unsettling brings about the type of expression that will contrast existing outcomes to demonstrate new effective and corrosion-resistive network structures. This model is especially disturbing as it deals with the geology of an HCP network in terms of numeric and graphical development and gives cautious outcomes. The review applied the irregularity index to find inconsistencies in the HCP network structure. After assessment, an ML-based Maple tool is utilized for the assertion and underwriting of results



Figure 1. HCI-Based methodology model

- To study a network, start by identifying nodes, edges, and network type. Choose an appropriate representation, such as an adjacency matrix or graph object. Choose topological invariants like degree distribution, clustering coefficient, average path length, betweenness centrality, and community structure. Use network analysis software like NetworkX, igraph, Gephi, or Maple. Visualize the network using tools like Gephi or Matplotlib to understand its structure.

- The study involves analyzing topological invariants to understand network features, such as power-law degree distributions and high clustering coefficients. It compares the network's invariants with similar networks to assess the relevance of the findings. Hypothesis testing is conducted to test the viability of specific hypotheses on the network's structure or behavior. The study is refined and iterative, focusing on specific network characteristics and evaluating the results in the context of the network's domain.
- To map HCP networks over a graph using topological invariants, establish the graph and identify the bridge nodes. Choose relevant invariants like degree centrality, betweenness centrality, closeness centrality, clustering coefficient, or community structure. Compute selected invariants for the graph's bridge nodes, examining connectedness and centrality. Map topological invariants to the corresponding graph bridge nodes, using visual encoding methods like color-coding or size variation.
- Display the underlying graph structure and map topological invariants using graph visualization tools or libraries. The study focuses on understanding the HCP network by examining mapped topological invariants and graph visualization. It refines the inquiry by examining additional features and comparing results with previous studies. The study validates the results by identifying important bridges based on their topological traits and discussing the network's consequences. In the future, the topological results will be optimized using optimization assistance tools.

Figure 2 shows a HCP network lattice which is a complex and symmetric structure, consisting of alternating layers of spheres of atoms stacked in a hexagon with a middle atom. The edge set E(G) connects the nearest atoms. In a 3D HCP (n), edges with filled and dotted lines are used to clarify bonding between atoms. The atoms in the middle layer share links with both hexagonal layers due to their symmetrical arrangement. Zirconium, ruthenium, hafnium, and other elements contribute to the formation of an HCP crystal structure. It is the most rigid and brittle form that is frequently seen in metals, and it encompasses a far wider range of metallic properties than a typical hexagonal crystal structure. It does not, however, have the same smooth symmetry as cubic structures.

Table 1 shows the edge partitions of the hexagonal closely packed network when converting into a graph after mapping mentioning cardinality with them. The vertex is a corner where the atom is attached and the edge is the length or bond between two atoms. The cardinality is the frequency of bonded edges. The study of several inorganic and organic chemical structures via graphical representation is possible thanks to chemical graph theory. Topological descriptors are mathematical concepts that correlate with chemical properties.



Figure 2. N unit cell hexagonal closely packed network lattice

Sr. No.	Edge representation	d _u , d _v	The cardinality of d _u , d _v	
1	E ₁	(5, 5)	12	
2	E_2	(5, 10)	12	
3	E ₃	(5, 8)	12	
4	E_4	(8, 8)	3n	
5	E_5	(8, 10)	6	
6	E_6	(7, 7)	12n-18	
7	E7	(7, 8)	12n-12	
8	E_8	(7, 14)	6n-6	
9	E ₉	(10, 14)	2	
10	E_{10}	(14, 14)	n-2	
11	E_{11}	(8, 14)	6n-6	
12	E_{12}	(5, 7)	12	

Table 1. Edg	e partitions of	of hexagonal	closely 1	packed net	twork graph	with cardinality
	, - r				0	

4. **RESULTS AND DISCUSSION**

The topological invariants from (1) to (10) are used to investigate the topology of the network graph of the HCP crystal structure. The "HCP" crystal network was mapped, transformed into a graph, solved, validated, and optimized to get the results presented in the methods section. Hexagonal closely packed lattice structure graph investigated by CQIs.

$$CQI(G) = \sum_{uv \in E(G)} \frac{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}{d_G(u) + d_G(v)}$$
(1)

$$QCI(G) = \sum_{uv \in E(G)} \frac{(d_G(u) + d_G(v))}{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}$$
(2)

$$KBSO(G) = \sum_{ue} \sqrt{d_u^2 + d_e^2}$$
(3)

KBSO_{re}d (G) =
$$\sum_{ue} \sqrt{(d_u - 1)^2 + (d_e - 1)^2}$$
 (4)

$$D(G) = \sum_{ue} \sqrt{du^3 + dv^3} \tag{5}$$

$$RD(G) = \sum_{ue} \sqrt{(du-1)^3 + (dv-1)^3}$$
(6)

$$KBRZ_1(HCP) = \frac{(d_u + d_\varrho)}{(d_u * d_\varrho)}$$
(7)

$$KBRZ_2(HCP) = \frac{(d_u + d_0)}{(d_u * d_0)}$$
(8)

$$KBRZ_{3}(HCP) = (d_{u} + d_{\varrho})(d_{u} * d_{\varrho})$$
⁽⁹⁾

$$ISO(G) = \sum_{ue} \sqrt{|d_u^2 - d_v^2|}$$
(10)

The (1) and (2) display the Contraharmonic-Quadratic index and Quadratic-Contraharmonic index, respectively. In (3) and (4) display the KBSO index and its reduced form. In (5) and (6) display the Dharwad index and the Reduced Dharwad index. In (7)-(9) display the First K-Banhatti Redefined Zagreb (KBRZ1) index, Second K-Banhatti Re Where "u" and "e" are the vertices of the graph HCP being discussed, du and de in the equations above are displaying edge partitions. The irregularity Sombor Index for revealing irregularities from the HCP network is represented by (10) at the conclusion.

4.1. Main results by CQIs

- Theorem 1

If HCP is a graph of a hexagonal closely-packed network used in alloys, aluminum lattice, zirconium lattice, and the fabrication of various chemical structures and utensils, then CQI and QCI solve as,

$$\begin{split} & CQI(G) = \sum_{uv \in E(G)} \frac{\sqrt{2(dc(u)^2 + dc(v)^2)}}{dc(u) + dc(v)} \\ & CQI(G) = \frac{\sqrt{2((5)^2 + (5)^2)}}{5+5} * 12 + \frac{\sqrt{2((5)^2 + (10)^2)}}{5+10} (12) + \frac{\sqrt{2((5)^2 + (8)^2)}}{5+8} (12) + \frac{\sqrt{2((8)^2 + (8)^2)}}{5+8} (3n) + \frac{\sqrt{2((8)^2 + (10)^2)}}{8+10} (6) + \frac{\sqrt{2((7)^2 + (7)^2)}}{7+7} (12n - 18) + \frac{\sqrt{2((7)^2 + (8)^2)}}{10+14} (2) + \frac{\sqrt{2((7)^2 + (14)^2)}}{7+14} (6n - 6) + \frac{\sqrt{2((10)^2 + (14)^2)}}{10+14} (2) + \frac{\sqrt{2((10)^2 + (14)^2)}}{8+14} (n - 2) + \frac{\sqrt{2((8)^2 + (14)^2)}}{8+14} (6n - 6) + \frac{\sqrt{2((5)^2 + (7)^2)}}{5+7} (12) \\ & CQI(G) = -8 + 4\sqrt{10} + \frac{12}{13}\sqrt{178} + 16n + \frac{2}{3}\sqrt{82} + \frac{1}{15}\sqrt{226} (12n - 12) + \frac{1}{3}\sqrt{10}(6n - 6) + \frac{7}{3}\sqrt{37} + \frac{1}{11}\sqrt{130}(6n - 6) \end{split}$$

- Theorem 2

Hexagonal closely packed lattice structure graph Investigated by QCI. Figure 3 outcomes represent sharp upper and lower limits (11) and (12) of CQ invariant and QC invariant when solving the topology of the

HCP network after mapping and their mathematical form will be used for the modeling of the more efficient and corrosion-resistive network structure.

$$\begin{aligned} QCI(G) &= \frac{5+5}{\sqrt{2((5)^2+(5)^2)}} * 12 + \frac{5+10}{\sqrt{2((5)^2+(10)^2)}} (12) + \frac{5+8}{\sqrt{2((5)^2+(8)^2)}} (12) + \\ &\frac{8+8}{\sqrt{2((8)^2+(8)^2)}} (3n) + \frac{8+10}{\sqrt{2((8)^2+(10)^2)}} (6) + \frac{7+7}{\sqrt{2((7)^2+(7)^2)}} (12n-18) + \\ &\frac{7+8}{\sqrt{2((7)^2+(8)^2)}} (12n-12) + \frac{7+14}{\sqrt{2((7)^2+(14)^2)}} (6n-6) + \frac{10+14}{\sqrt{2((10)^2+(14)^2)}} (2) + \\ &\frac{14+14}{\sqrt{2((14)^2+(14)^2)}} (n-2) + \frac{8+14}{\sqrt{2((8)^2+(14)^2)}} (6n-6) + \frac{5+7}{\sqrt{2((5)^2+(7)^2)}} (12) \\ &QCI(G) &= -8 + \frac{18}{5} \sqrt{10} + \frac{78}{89} \sqrt{178} + 16n + \frac{27}{41} \sqrt{82} + \frac{15}{226} \sqrt{226} (12n-12) + \\ &\frac{3}{10} \sqrt{10} (6n-6) + \frac{84}{37} \sqrt{37} + \frac{11}{130} \sqrt{130} (6n-6) \end{aligned}$$

4.2. Main results by KBSO Indices

- Theorem 3

If HCP is a graph of the hexagonally closely packed network used to make alloys, the aluminum lattice, the zirconium lattice, as well as various chemical structures and utensils, then KBSO and KBSOred indices are solving as follows,

$$KBSO(G) = \sum_{ue} \sqrt{d_{u}^{2} + d_{\varrho}^{2}}$$

the (13) shows the k-banhatti sombor index which will be used for the solution of HCP mentioned in Figure 2.

$$KBSO_{r\varrho}\underline{d}(G) = \sum_{ue} \sqrt{(d_{u} - 1)^{2} + (d_{\varrho} - 1)^{2}}$$

The (14) shows the k-banhatti sombor reduced index which will be used for the solution of the HCP network mentioned in Figure 2.

$$\begin{aligned} & KBSO(G) = \sqrt{5^2 + 8^2} (12) + \sqrt{5^2 + 13^2} (12) + \sqrt{5^2 + 11^2} (12) + \sqrt{8^2 + 14^2} (3n) + \\ & \sqrt{8^2 + 16^2} (6) + \sqrt{7^2 + 12^2} (12n - 18) + \sqrt{7^2 + 13^2} (12n - 12) + \sqrt{7^2 + 19^2} (6n - 6) + \sqrt{10^2 + 22^2} (2) + \sqrt{14^2 + 26^2} (n - 2) + \sqrt{8^2 + 20^2} (6n - 6) + \sqrt{5^2 + 10^2} (12) \\ & KBSO(G) = 12\sqrt{89} + 12\sqrt{194} + 16\sqrt{146} + 6\sqrt{65} (n) + 108\sqrt{5} + \sqrt{193} (12n - 18) + \\ & \sqrt{218} (12n - 12) + \sqrt{410} (6n - 6) + 2\sqrt{218} (n - 2) + 4\sqrt{29} (6n - 6) \end{aligned}$$
(13)

- Theorem 4

$$\begin{aligned} & KBSOred(G) = \sqrt{4^2 + 7^2} (12) + \sqrt{4^2 + 12^2} (12) + \sqrt{4^2 + 10^2} (12) + \sqrt{7^2 + 13^2} (3n) + \\ & \sqrt{7^2 + 15^2} (6) + \sqrt{6^2 + 11^2} (12n - 18) + \sqrt{6^2 + 12^2} (12n - 12) + \sqrt{6^2 + 18^2} (6n - 6) + \sqrt{9^2 + 21^2} (2) + \sqrt{13^2 + 25^2} (n - 2) + \sqrt{7^2 + 19^2} (6n - 6) + \sqrt{4^2 + 9^2} (12) \\ & KBSOred(G) = 12\sqrt{65} + 48\sqrt{10} + 24\sqrt{29} + 3\sqrt{218} (n) + 6\sqrt{274} + \sqrt{157} (12n - 18) + \\ & 6\sqrt{5} (12n - 12) + 6\sqrt{10} (6n - 6) + 6\sqrt{58} + \sqrt{794} (n - 2) + \sqrt{410} (6n - 6) + 12\sqrt{97} \end{aligned}$$
(14)

Figure 4 outcomes represent sharp upper and lower limits in (13) and (14) of KBSO invariants and their decreased form when solving the topology of the HCP network after mapping and their mathematical form will be used for the modeling of the more efficient and corrosion-resistive network structure.

4.3. Main results by Dharwads indices

- Theorem 5

Let HCP be a graph of the hexagonal closely-packed network used in alloys, aluminum lattice, and zirconium lattice and for making different chemical structures and utensils also, then, Dharwad and Dharwadred indices are solving as:

$$\begin{split} D(G) &= \sum_{ue} \sqrt{du^3 + dv^3} \\ D(HCP) &= \sqrt{5^3 + 5^3} (12) + \sqrt{5^3 + 10^3} (12) + \sqrt{5^3 + 8^3} (12) + \sqrt{8^3 + 8^3} (3n) + \\ \sqrt{8^3 + 10^3} (6) + \sqrt{7^3 + 7^3} (12n - 18) + \sqrt{7^3 + 8^3} (12n - 12) + \sqrt{7^3 + 14^3} (6n - 6) + \sqrt{10^3 + 14^3} (2) + \sqrt{14^3 + 14^3} (n - 2) + \sqrt{8^3 + 14^3} (6n - 6) + \sqrt{5^3 + 7^3} (12) \\ D(HCP) &= 60\sqrt{10} + 180\sqrt{5} + 156\sqrt{13} r + 96n + 36\sqrt{42} + 7\sqrt{14} (12n - 18) + \\ 3\sqrt{95} (12n - 12) + 21\sqrt{7} (6n - 6) + 24\sqrt{26} + 28\sqrt{7} (n - 2) + 2\sqrt{814} (6n - 6) \end{split}$$
(15)

Theorem 6

$$\begin{aligned} RD(G) &= \sum_{ue} \sqrt{(du-1)^3 + (dv-1)^3} \\ RD(HCP) &= \sqrt{4^3 + 4^3} (12) + \sqrt{4^3 + 9^3} (12) + \sqrt{4^3 + 7^3} (12) + \sqrt{7^3 + 7^3} (3n) + \\ \sqrt{7^3 + 9^3} (6) + \sqrt{6^3 + 6^3} (12n-18) + \sqrt{6^3 + 7^3} (12n-12) + \sqrt{6^3 + 13^3} (6n-6) + \sqrt{9^3 + 13^3} (2) + \sqrt{13^3 + 13^3} (n-2) + \sqrt{7^3 + 13^3} (6n-6) + \sqrt{4^3 + 6^3} (12) \\ RD(HCP) &= 6144 + 12\sqrt{793} + 12\sqrt{407} + 21\sqrt{14} n + 24\sqrt{67} + 12\sqrt{3} (12n-18) + \\ \sqrt{559} (12n-12) + \sqrt{2413} (6n-6) + 2\sqrt{2926} + 13\sqrt{26}(n-2) + 2\sqrt{635}(6n-6) + 24\sqrt{70} \end{aligned}$$
(16)

Figure 5 outcomes represent sharp upper and lower limits in (15) and (16) of the Dharwad invariant and their decreased form when solving the topology of the HCP network after mapping. Their mathematical form will be used for the modeling of the more efficient and corrosion-resistive network structure. There graphical simulated results show lower and upper bounds of the network.

4.4. Main results by KBRZ Indices

- Theorem 7

Let HCP be a graph of the hexagonal closely-packed network used in alloys, aluminum lattice, and zirconium lattice and for making different chemical structures and utensils also, then, $KBRZ_1$, $KBRZ_2$, and $KBRZ_3$ indices are solving as (17).

$$\begin{aligned} KBRZ_{1}(HCP) &= \frac{5+8}{5*8} * 12 + \frac{5+13}{5*13} (12) + \frac{5+11}{5*11} (12) + \frac{8+14}{8*14} (3n) + \frac{8+16}{8*16} (6) + \\ &\frac{7+12}{7*12} (12n - 18) + \frac{7+13}{7*13} (12n - 12) + \frac{7+19}{7*19} (6n - 6) + \frac{10+22}{10*22} (2) + \frac{14+26}{14*26} (n - 2) + \frac{8+20}{8*20} (6n - 6) + \frac{5+10}{5*10} (12) \\ &KBRZ_{1}(HCP) = \frac{5004577}{760760} + \frac{572213}{69160} (n) \end{aligned}$$
(17)

Figure 6 outcomes represent sharp upper and lower limits in (17) of FKBRZ invariant when solving the topology of the HCP network after mapping. Their mathematical form will be used for the modeling of the more efficient and corrosion-resistive network structure. There graphical simulated results show lower and upper bounds of the network.







Empowered corrosion-resistant products through HCP crystal network ... (Khalid Hamid)



Figure 5. Hexagonal closely packed lattice structure graph investigated by Dharwad and reduced Dharwad invariants



Figure 6. Hexagonal closely packed lattice structure graph investigated by First K-Banhatti Redefined Zagreb (FKBRZ) index

- Theorem 8

$$\begin{aligned} KBRZ_{2}(HCP) &= \frac{5*8}{5+8} * 12 + \frac{5*13}{5+13} (12) + \frac{5*11}{5+11} (12) + \frac{8*14}{8+14} (3n) + \frac{8*16}{8+16} (6) + \\ &\frac{7*12}{7+12} (12n - 18) + \frac{7*13}{7+13} (12n - 12) + \frac{7*19}{7+19} (6n - 6) + \frac{10*22}{10+22} (2) + \frac{14*26}{14+26} (n - 2) + \frac{8*20}{8+20} (6n - 6) + \frac{5*10}{5+10} (12) \\ &KBRZ_{2}(HCP) = -\frac{261958}{25935} + \frac{37468073}{190190} (n) \end{aligned}$$
(18)

Figure 7 outcomes represent sharp upper and lower limits in (18) of SKBRZ invariant when solving the topology of the HCP network after mapping. Their mathematical form will be used for the modeling of the more efficient and corrosion-resistive network structure. There graphical simulated results show lower and upper bounds of the network.

Figure 8 outcomes represent sharp upper and lower limits in (19) of TKBRZ invariant when solving the topology of the HCP network after mapping. Their mathematical form will be used for the modeling of the more efficient and corrosion-resistive network structure. There graphical simulated results show lower and upper bounds of the network.

- Theorem 9

$$\begin{split} & KBRZ_{3}(HCP) = (5+8)x5x8x12 + (5+13)x5x13x (12) + (5+11)x5x11x(12) + \\ & (8+14)x8x14x(3n) + (8+16)x8x16x(6) + (7+12)x7x12x(12n-18) + \\ & (7+13)x7x13x(12n-12) + (7+19)x7x19x(6n-6) + (10+22)x10x22x(2) + \\ & (14+26)x14x26 (n-2) + (8+20)x8x20x(6n-6) + (5+10)x5x10x(12) \\ & KBRZ_{3}(HCP) = -54964 + 110572(n) \end{split}$$

4.5. Main results by ISO index for irregularities

Let HCP be a graph of the hexagonal closely-packed network used in alloys, aluminum lattice, and zirconium lattice and for making different chemical structures and utensils also, then, the ISO index is used to find the irregularities from the concerned network as,

- Theorem 10

$$ISO(G) = \sum_{ue} \sqrt{|d_u^2 - d_v^2|}$$

$$ISO(HCP) = \sqrt{|5^2 - 5^2|} (12) + \sqrt{|5^2 - 10^2|} (12) + \sqrt{|5^2 - 8^2|} (12) + \sqrt{|8^2 - 8^2|} (3n) + \sqrt{|8^2 - 10^2|} (6) + \sqrt{|7^2 - 7^2|} (12n - 18) + \sqrt{|7^2 - 8^2|} (12n - 12) + \sqrt{|7^2 - 14^2|} (6n - 6) + \sqrt{|10^2 - 14^2|} (2) + \sqrt{|14^2 - 14^2|} (n - 2) + \sqrt{|8^2 - 14^2|} (6n - 6) + \sqrt{|5^2 - 7^2|} (12)$$

$$ISO(HCP) = 36 + 60\sqrt{3} + 12\sqrt{39} + \sqrt{15} (12n - 12) + 7\sqrt{3} (6n - 6) + 32\sqrt{6} + 2\sqrt{33} (6n - 6)$$
(20)

HCI provided the mapping framework and modern topological invariants to solve the existing network HCP used in different products and alloys for corrosion resistance concerns. The mathematical deduced results under the umbrella of HCI improve the effectiveness of alloys regarding corrosion resistivity by indulging best characteristics with the help of modeling of HCP networks as these are used in alloy products. In (11)-(20) will be used for the modeling of HCP networks and also provide guidelines for the engineers and manufacturers.



Figure 7. Hexagonal closely packed lattice structure graph investigated by Third K-Banhatti Redefined Zagreb (TKBRZ) index



Figure 8. Hexagonal closely packed lattice structure graph investigated by Second K-Banhatti Redefined Zagreb (SKBRZ) index

4.6. Applications

This study presents a novel direct interconnection network model using graphs to represent processors and connections. It explores addressing and routing techniques for topological characteristics like degree, node and edge symmetry, and surface area. Regular polygons like triangular, square, and hexagonal are used to create efficient direct connectivity networks. Mesh-connected computers and tori are well-known and widely used models for parallel processing that are based on ordinary square tessellations. Tori meshed processors in higher dimensions, utilizing the Mary K-cube extension in practical multi-computers like J-machine, iWarp, Ncube-2, Cray T3E, and Cray T3D.

Topological descriptors are mathematical concepts that correlate with chemical properties. HCP is a complex and symmetric structure, consisting of alternating layers of spheres of atoms stacked in a hexagon with a middle atom. The edge set E(G) connects the nearest atoms. In a 3D HCP (n), edges with filled and dotted lines are used to clarify bonding between atoms. The atoms in the middle layer share links with both hexagonal layers due to their symmetrical arrangement. Also described are straightforward embeddings between two networks. In other words, we demonstrate how to maintain the simplicity of fundamental data transmission algorithms like routing and broadcasting while reducing the dimension of a mesh by eliminating some nodes and turning it into a hexagonal network.

5. CONCLUSION

HCI is a science that aims to empower product users by improving the effectiveness and efficiency of the apps and products they use with the help of TIs. This study investigates the crystal structures used in alloys and how they can be improved for corrosion resistance. Metals and alloys are susceptible to corrosion, despite technological advances in processing that have improved their performance. When a pure metal or alloy comes into contact with its surroundings, a natural process takes place that converts it into the thermodynamically preferred oxide, hydroxide, carbonate, or sulphide. As a result, the material gradually degrades and disintegrates, potentially leading to a loss of functionality, structural collapse, or even environmental contamination from the discharge of potentially hazardous substances, as well as decreased efficiency and effectiveness. In the study, HCI identifies requirements that emphasize examining an existing HCP network for requirements in the form of vertices and edges, mapping different vertices and edges of the network graph with topological invariants, solving the network graph using invariants, and providing results for modeling and design of advanced networks and architectures. The HCI also ensures and investigates the optimization of specifications-compliant results. The results are also checked to meet the requirements, for this purpose, the study examined the network graph results for irregularities and produced results of irregularities against the given network graph. The mathematical and graphical results provide guidelines for engineers and manufacturers through modeling by getting advanced architectures of alloys with characteristics. Chemical and physical properties are directly related to the dimensions and topologies of a network used in alloys.

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