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Article

Influential Yield Strength of Steel Materials with Return Random Walk Gravity Centrality

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Abstract: In complex networks, important nodes have a significant impact, both functional and structural. From the perspective of data flow pattern detection, the evaluation of the importance of a node in a network, taking into account the role it plays as a transition element in random paths between two other nodes, has important applications in many areas. Advances in complex networks and improved data generation are very important for the growth of computational materials science. The search for patterns of behavior of the elements that make up steels through complex networks can be very useful in understanding their mechanical properties. This work aims to study the influence of the connections between the elements of steel and the impact of these connections on their mechanical properties, more specifically on the yield strength. The patterns found in the results show the significance of the proposed approach for the development of new steel compositions.

Keywords: centrality measure; complex networks; random walk; steel materials

MSC: 74A40

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1. Introduction

In recent years, the area of complex networks has gained importance in several scientific fields to help in the comprehension of interconnected elements, such as biology, social networks, urban mobility, and medicine [1–4]. Moreover, in complex networks, the interaction between the vertices follows various kinds of patterns that can include all different relationships [5]. The exchange of ideas or diseases, the transmission of information, and the influence between interconnected vertices are fundamental aspects of intricate networks. Consequently, assessing the impact of nodes within a network is a particularly significant subject for comprehending phenomena like the dissemination of information in a network, based on the importance of a vertex within it [6–10].

One of these fields is materials science, where the study of the mechanical properties of steel has a history of approaches based on machine learning and data science. The emergence of computational databases has made integration, analysis and prediction a key issue in the investigation of the mechanical properties of steels and their relationship with their composition [11]. In this way, the advances in complex networks and improved data generation have created fertile ground for computational materials science. Thus, the combination of complex networks through centrality measures, together with the study of the mechanical properties of steels by means of their composition is especially useful to promote progress in this science. This is what warrants the presentation of this paper.

This work focuses on studying behavior patterns of the connections between the elements of the steels and the influence of these connections on their mechanical properties,

more specifically on yield strength. For this purpose, we apply an analysis, based on complex networks, with a measure of centrality that takes into account the static and dynamic interactions of a network. Classical centrality measures have been widely studied and have many applications in a multitude of networks, however, most network problems resist a standard solution and require a particular solution through the adaptation or creation of a specific centrality measure. The centrality measure created or adapted arises from the in-depth study of the network as well as the interactions between the nodes that form it.

2. Related Work

Nowadays, digital technologies and the ease of access to a lot of datasets acquired from different sources have heightened the enthusiasm for investigating the structural attributes of networks that mirror authentic challenges and exhibit intricate characteristics. The assortment of techniques, principles, algorithms, and models advanced are useful for analyzing the structure of the makeup of real networks and has established the foundation of what is commonly referred to as complex network theory [12–15].

In order to delineate and grasp the role of a vertex within a complex network, the widespread practice is to employ centrality metrics. Within the realm of investigating the attributes and significance of a component (node) within a complex network, there exists a wide array of metrics available for examination, encompassing both local and global approaches [16–18].

There are techniques, specifically labeled as betweenness centrality measures, which assess a node's significance by considering network flow dynamics, primarily focusing on the network's operation concerning the shortest path perspective [19]. However, certain issues cannot be adequately addressed through the shortest path approach, as they necessitate an understanding of the connectivity characteristics within both static and dynamic networks. To gain insights into these types of networks, in [20], the author introduced a measure for undirected networks that amplifies the importance of nodes within densely connected clusters. Additionally, in [21], an examination of node properties in directed networks is presented, with potential applications in various domains such as social media, mobility, and materials science, among others.

The authors propose some measures in [22,23] to study the influence of neighboring nodes and those within a specific radius. Nevertheless, many real-world networks exhibit dynamic topological properties and structures that identify relevant information from important nodes. In addressing this, the concept of effective distance shown in [24] aids in uncovering hidden dynamic insights.

In [25], a novel centrality measure is introduced, which combines elements like a walk-based link predictor (Return Random Walk, RRW), effective distances, and a gravity model. This metric serves a dual purpose: at a local level, the vertices are significant based on their relevance within their community/cluster. At the same time, at a global level, this measure contributes to enhancing network cohesion. The strength of this approach lies in its ability to detect crucial vertices by combining both static and dynamic information. The use of these kinds of walks (RRW) enables the highlighting of community structures while considering a blend of global and local data [26].

On the other hand, steel is one of the most widely used materials worldwide, which means that almost all countries have specific regulations to guarantee its quality since it has a direct impact on the industrial, construction, and economic sectors. At the international level, ISO standards are established by the International Organization for Standardization (ISO), and in these standards steel can be found in the "P" classification within the groups of general materials. Steel is made up of iron and carbon, the second component being present in percentages between 0.008% and 0.2%, although other accessory elements such as silicon, phosphorus, manganese, sulfur, oxygen, etc., are also normally present. There are currently more than 5000 variations of steel created from the combination of these elements with alloying elements which, when added, give them different characteristics.

The composition of steels is a key factor in their behavior, as well as their microstructure based on their composition, heat treatments, mechanical processes, etc. There are many studies that try to clarify the relationship between the chemical composition of steel and its mechanical properties [27,28]. These studies show how the composition of steel (iron, carbon, sulfur, phosphorus, silicon, manganese, carbon equivalent, copper, etc.) affects its yield strength and tensile strength. The yield strength is the key parameter for engineers when establishing failure criteria in ductile materials, since once exceeded the material begins to be considered plastically deformed and therefore does not retain the ideal properties in the performance of its engineering function. The optimization of steel composition has been, and is, widely studied [29,30], however neural network studies rarely focus on it. In this connection, many recent studies on steels try to explain the connection between composition and mechanical properties by using machine learning or neural networks, among others [11,31–33].

The present research focuses on the novel study of understanding the impact of steel composition on the mechanical properties of steels through the application of graph theory, in particular centrality measures. The study attempts to address the importance of the connections between the elements and the influence of these connections on their mechanical properties, more specifically on yield strength. Our proposal focuses on the analysis of a particular family of steels, structural steels, which are designed for the construction of building structures and machinery components. This steel can be in the form of rolled sections, reinforced members, or steel-concrete composite sections in the construction of urban buildings.

In summary, the aim of this research is to identify the influence on the yield strength of the connections between the different chemical elements that make up the structural steels analyzed. To address this objective, the article is divided into a methodology (Section 3) which includes the adapted centrality measure chosen, Section 4 with the explanation of the database, the creation of the network of chemical elements that make up the structural steels analyzed, and the results of our experiments. Finally, the discussion (Section 5) and conclusions (Section 6) of this research are presented to conclude this research.

3. Methodology

In this section, the centrality measure used to obtain a ranking that lets us study the process of construction of the steel network is presented.

To analyze the steel network, in this paper, we use a novel algorithm of centrality measure that combines three concepts:

1. The effective distances: It is used to catch the static and dynamic data of the topology of a network.
2. The gravity concept: It measures the power of attraction of a node into the network.
3. The return random walks algorithm: It identifies the strength or weakness of all nodes of the network.

In this respect, the Return Random Walk Gravity Centrality algorithm [25] (RRWG) focuses on the problem of influential node identification in real networks considering the local (intra-cluster) and the global information (inter-cluster) of a network. This approach captures the static and dynamic interactions –links– of a network, detecting the nodes that strengthen the network from a dense clusters perspective. It is necessary to point out that this centrality measure works for both directed and undirected networks.

The effectiveness and robustness of the RRWG algorithm is proved in [25]. In this paper, the authors used seven real networks (directed, undirected, weighted, and unweighted) and, using the SIR model, they compared the RRWG metric with seven centrality measures (classical and current), obtaining very successful results.

This metric obtains good results for the propagation and detection of the most influential nodes in networks, working more effectively in dense networks, avoiding the limitation of the unreachable end nodes due to the properties of the approach.

The aforementioned measure is inspired by the gravitational law, the effective distance and it incorporates dynamic information containers in the topology of the network. It is given by the expression

$$C_{EffG}(i) = \sum_{j=1, j\neq i}^{N} \frac{K_i K_j}{D_{j|i}^2}, \tag{1}$$

where N in the number of nodes, K_i and K_j are the degree of the nodes i and j respectively, and $D_{j|i}$ is the effective distance between nodes i and j

$$D_{j|i} = 1 - log_2\left(\frac{a_{ij}}{K_i}\right). \tag{2}$$

with a_{ij} the element ij of the adjacency matrix. Thus, the gravity centrality of node i can be estimated following Equation (1) above.

It should be noted that the effective distance is not defined for isolated nodes, or rather, it can be considered infinite for isolated nodes. As a consequence, the centrality measure defined in Equation (1) is not defined for isolated nodes.

The main contribution of this measure is to increase the relevance of the nodes from a double point of view: on the one hand, it combines static and dynamic information through the effective distances in a gravity model and, on the other hand, the use of return random walk reinforces the community structure, considering both global and local information (increasing the centrality of the relevant nodes in reinforcing their community).

In summary, this method is appropriate for studying the betweenness information of a dense network.

4. Experiment Results

Firstly, the dataset employed and the formation of the steel network are explained in detail. Then, we show the results of the experiments, comparing the RRWG method with the classical betweenness centrality.

4.1. Dataset

This study analyses the influence of the variation in the percentages of chemical elements in structural steels as well as the influence of the presence of these elements on such a relevant variable as yield strength. The yield strength is an intrinsic property of each material and has served as a failure criterion for materials considered to have ductile behavior, since once its value is exceeded, the deformations in the material are permanent, and therefore the material loses its structural integrity.

To analyze the influence of the elements as well as the percentage of the same in steels, we have created our database, which includes so-called structural steels (following ISO standards). Furthermore, these steels selected and included in the database have been subjected to the same rolling process, with temperatures above 0–30 ÂºC , their geometry is in the form of plates and all the steels have been subjected to static tensile tests from which the fundamental variable of the study, the yield strength, has been obtained. In [34], readers can consult the database created of the structural steels (a total of 90) as well as the elements that make them up (17), and their percentages.

All the information on the structural steels that make up the new dataset https://github.com/manucurado/steels (accessed on 25 January 2024) have been extracted from the prestigious Total Material Database (see [34]). This database is one of the most extensive worldwide with more than 20,000,000 proprietary records for more than 450,000 metallic and non-metallic materials, as well as international cross-referencing for 450,000 materials from 74 standards.

4.2. Steel Network Construction

In this section, the methodology followed for the creation of the network is presented. It should be pointed out that a toy example is built with the idea of simplifying the

understanding of the creation of the network. In addition, as previously mentioned, we start from an already created steel database.

Firstly, the graph is generated by defining the variables of the graph $G = (V, E, W)$ where V—nodes—are the different alloy compositions of the structural steels considered, E—edges—are the relationships between the nodes, between steels sharing chemical elements, and W is the weight of the edges. In our network, this weight will be represented by a characteristic parameter to be analyzed: the value of the weighted yield strength σ_Y.

To achieve the objective of this study and to analyze the influence of the alloy chemical elements and their relationships on the yield strength, a directed graph is generated. Note that a direct graph has connections and weights in both directions between each two related nodes—steels. This choice is justified by the suitability of the behaviour of the connections between the alloy chemical elements that make up the steels, in the same way as happened in the elaboration of graphs to evaluate the influence of chemical elements in the formation of glassy materials, as reported in recent research [35].

Being a directed graph, there shall be an incoming and an outgoing edge for each node—steel. Given two alloy compositions of steels A_i and A_j, with their respective compositions (alloy chemical elements), the formation of the network requires the following steps:

4.2.1. Step 1: Common (IN)

The weight of the outgoing edge—from steel A_j to steel A_i—is the sum of the minimum percentages of each chemical element shared by both steels multiplied by the yield strength of the starting steel A_j.

$$A_j \rightarrow A_i = \sigma_{Y_j} \sum_{\forall k \in Z_{ij}} \min(e_{i_k}, e_{j_k}), \tag{3}$$

where $\min(e_{i_k}, e_{j_k})$ is the minimum percentage of the shared element in both steels and σ_{Y_j} is the yield strength of the source steel A_j, and Z_{ij} is the set of common elements of i and j.

Figure 1 shows two compositions of steels A_1 and A_2 with alloys compositions:

$$Al0.15Mn0.2Cu0.3 \text{ and } Al0.5Mn0.35P0.02.$$

4.2.2. Step 2: Differences (OUT)

The weight of the outgoing edge from steel A_i to steel A_j is the sum of the percentages exceeding each common chemical element multiplied by the yield strength of the source steel A_i.

$$A_j \leftarrow A_i = \sigma_{Y_i} \sum_{\forall k \in Z_{ij}} excess(e_{i_k}), \tag{4}$$

where $\text{excess}(e_{i_k})$ is the percentage excess of common element k in material A_i with respect to A_j and σ_{Y_i} is the yield strength of the source material A_i, and Z_{ij} is the set of common elements of i and j.

In the toy example of Figure 1, the outgoing alloy composition steel A_1 has 0.15% of Al and the incoming alloy composition steel A_2 has 0.5% then, the excess of the aluminium of this edge will be 0.10%. On the other hand, the case of Mn is, using the same procedure, 0%, since from steel A_1 to A_2 there is no excess of this common chemical element. If we add the excess percentages of the two common alloy elements, Mn, and Al, and multiply it by the yield strength of steel A_1, we will obtain the value of the weight of the edge, in this case (0.10% + 0%) multiplied by 220 MPa.

4.2.3. Step 3: Create the Network

From a dataset with 90 different structural steel materials, and calculating the edge weights as explained in the previous steps, we construct a single weighted directed graph G, which represents the relationship between the materials from the perspective of the shared elements and their yield strength. Edges, connections between nodes, will only exist between steels that share chemical elements.

In total, the new graph has 7301 edges. This dense network is suitable for calculating the importance of each material with random-return gravity centrality. The weighted matrix is calculated from all the relationships between each pair of steel compositions A_i and A_j, by means of the following equation:

$$W_{ij} = A_i(\text{OUT}) + A_j(\text{IN}), \tag{5}$$

and

$$W_{ji} = A_j(\text{OUT}) + A_i(\text{IN}), \tag{6}$$

Applying this third step to the toy example, the outgoing edge of steel A_1 to A_2 will have a total weight of the sum of the total of the same outgoing edge of the differences plus the incoming edge of commons both from alloy compositions steel A_1 to A_2. Similarly, the outgoing edge from steel A_2 to A_1 will have a total weight of the sum of the total of the same outgoing edge of the commons plus the incoming edge of differences both from steel A_2 to A_1. The result of the total weight of the edges forming the network between steel A_1 and A_2 of the directed network is shown at the end of Figure 1. In this figure we show a toy sample of constructing the network from two structural steels that share two alloy elements: aluminium (Al) and manganese (Mn).

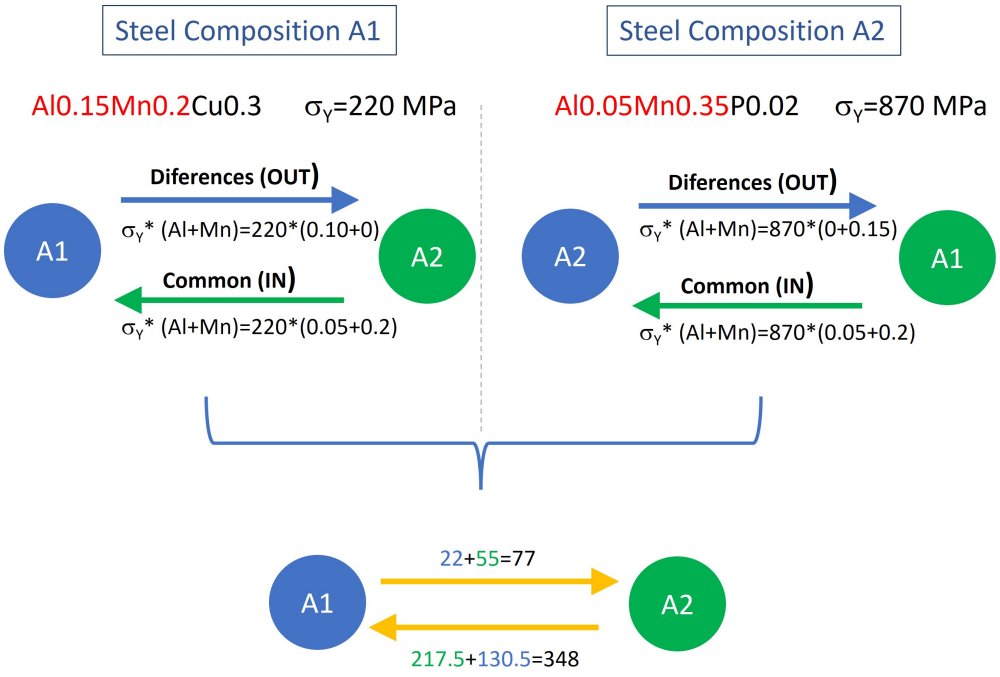

Figure 1. Toy sample: construction of the network with fictitious alloy compositions steels. Green color means the minimum amount of elements shared between nodes, and blue color means the excess of elements that could be shared from origin to destination material composition. Note that the alloy elements copper (Cu) and phosphorus (P) do not affect the network as they are not shared in both steels considered, and the sum of the percentage is not 100% as only the composition of the alloy elements is shown.

The resulting network is a graph G = (V, E, W), where V = 90 is the number of steel composition materials selected, E = 7301 is the number of edges of the network, that represent the relationships between steel materials in terms of chemical element ratio shared and the yield strength (see Table 1).

Note that the global density of the network is 89.14%. Because of this, the network is an almost complete graph. In this type of graph the visual representation does not contribute anything.

Table 1. Static network Information.

Nodes	Edges	Density	Avg. Degree	Max. Degree
90	7301	89.14%	43.27	92

4.3. Results

The following section includes the results of the steels with the most influential ratios for yield strength improvement, both using the classical betweenness centrality measure and the centrality measure proposed by Return Random Walk Gravity.

4.3.1. Classic Betweenness Centrality

The betweenness centrality measures (CBT) are based on the relevance of the shortest paths and the random path, i.e., they measure the global importance of a node as an intermediate node, but they have the common characteristic of not taking into account the cluster density of each node. However, to make a comparison and ratify the results with the chosen centrality measure, the ten structural steels with the best combination of elements in terms of their contribution to the improvement of the yield strength parameter are listed in Table 2.

The results show that the best combination of elements is between manganese, phosphorus, and sulfur as well as silicon to a lesser extent. The betweenness centrality measures the overall importance of a node as an intermediate node but havs the common feature of not taking into account the cluster density of each node. Therefore it does not give good results to apply the centrality measure in such dense networks and with the main objective listed. It is thus clear that steels with such an almost exclusive combination of these elements have low yield strength values.

Table 2. Top-10 ranking of steel materialsconcerningo element sharing with classical betweenness centrality.

Ranking	Material	Yield Strength	Composition (%)
1	Fe490*	275	C(0.21) Mn(1.5) P(0.03) S(0.05)
2	FeE355*	355	C(0.12) Mn(1.65) P(0.03) S(0.003)
3	E235B*	225	C(0.17) Mn(1.4) P(0.045) S(0.045) Si(0.4)
4	Fe430B*	215	C(0.21) Mn(1.5) P(0.045) S(0.045) Si(0.4)
5	TCR220 Class D*	220	C(0.15) Cr(0.15) Cu(0.2) Mo(0.06) N(0.09) Nb(0.08) Ni(0.02) P(0.035) S(0.035) Ti(0.008) V(0.008)
6	TCR220 Class B*	220	C(0.15) Cr(0.15) Cu(0.2) Mo(0.06) N(0.015) Nb(0.08) Ni(0.02) P(0.035) S(0.035) Ti(0.008) V(0.008)
7	C10D2	154	Al(0.01) C(0.1) Cr(0.1) Cu(0.15) Mn(0.4) Mo(0.05) N(0.007) Ni(0.1) P(0.02) S(0.025) Si(0.3) V(0.075)
8	R28*	155	C(0.1) Mn(0.3) P(0.04) S(0.04)
9	C25E4*	230	C(0.255) Mn(0.45) P(0.035) S(0.035) Si(0.25)
10	C10*	250	C(0.1) Mn(0.6) P(0.035) S(0.035) Si(0.4)

4.3.2. RRWG Centrality Evaluation

Taking into account that an analysis of steel materials to identify the most relevant materials according to their yield strength is performed, we need to apply an algorithm that helps us to rank the most influential nodes with respect to the local and global information of their relationships (common elements rate and yield strength). Thus, once the database of structural steels had been created, the Return Random Walk Gravity Centrality—expression (1)—is applied. The results obtained, in terms of ranking, are shown in Table 3.

This table shows the materials from the highest to lowest positions in the ranking of the centrality measure calculation, as well as their yield strength and chemical composition. The positions occupied in this ranking show the greater influence of the combinations of chemical elements within each steel on the yield strength. In other words, the higher the ranking position obtained, the more influential the combination of alloying chemical elements is in terms of producing an improvement in yield strength.

Table 3. Top-10 Ranking comparison, based on RRWG, of steel material network with respect the elements sharing.

Ranking	Material	Yield Strength	Composition (%)
1	DP600 Type 2*	600	B(0.005) C(0.2) Cr(0.15) Cu(0.2) Mn(0.3) Mo(0.06) Nb(0.008) Ni(0.2) P(0.03) S(0.03) Si(1.4) Ti(0.008) V(0.008)
2	P460QL2*	400	B(0.005) C(0.18) Cr(0.5) Cu(0.3) Mn(1.7) Mo(0.5) N(0.015) Nb(0.05) Ni(1) P(0.02) S(0.005) Si(0.5) Ti(0.03) V(0.08) Zr(0.05)
3	C20D2	622	Al(0.01) C(0.205) Cr(0.1) Cu (0.15) Mn(0.4) Mo(0.05) N(0.007) Ni(0.1) P(0.02) S(0.025) Si(0.3) V(0.075)
4	46Cr2*	873	Al(0.007) C(0.46) Cr(0.5) Cu(0.25) Mn(0.65) P(0.025) S(0.025) Si(0.3)
5	P355M*	345	Al(0.02) C(0.14) Mn(1.6) Mo(0.2) N(0.015) Nb(0.05) Ni(0.5) P(0.025) S(0.01) Si(0.5) Ti(0.05) V(0.1)
6	C8D2	892	Al(0.01) C(0.08) Cr(0.1) Cu(0.15) Mn(0.4) Mo(0.05) N(0.007) Ni(0.1) P(0.02) S(0.025) Si(0.3) V(0.075)
7	P355ML1*	345	Al(0.02) C(0.14) Mn(1.6) Mo(0.2) N(0.015) Nb(0.05) Ni(0.5) P(0.02) S(0.008) Si(0.5) Ti(0.05) V(0.1)
8	P355ML2*	345	Al(0.02) C(0.14) Mn(1.6) Mo(0.2) N(0.015) Nb(0.05) Ni(0.5) P(0.02) S(0.005) Si(0.5) Ti(0.05) V(0.1)
9	C7D	696	Al(0.01) C(0.07) Cr(0.2) Cu(0.3) Mn(0.25) Mo(0.05) Ni(0.25) P(0.035) S(0.035) Si(0.3) V(0.075)
10	Grade CR1*	210	C(0.15) Cr(0.15) Cu(0.2) Mn(0.6) Mo(0.06) Nb(0.008) Ni(0.2) P(0.05) S(0.035) Ti(0.008) V(0.008)

The analyzed results show that the four top-ranked structural steels possess combinations of the chemical elements Chromium (Cr), Copper (Cu), and Manganese (Mn).

Analyzing the first nine best-ranked structural steels, there are common combinations of chemical elements, phosphorus (P), sulphur (S), and silicon (Si).

In addition, among the percentages of the different elements that make up these steels, it should be noted that the most significant value of the steel that occupies the first position in the ranking is silicon, showing a percentage of 1.4 (%). Within the analysis, it is worth highlighting the relevance of the absence of the chemical element silicon in the structural steels analysed; only one of the 10 structural steels with the worst positions in the classification shows a percentage of it. The relationship of the rest of the key chemical elements listed with Si is key to the improvement of the yield strength.

On the other hand, and only failing to comply with this combination in the steel that occupies the fourth position in the ranking, similar connections are shown between the chemical elements, molybdenum (Mo), nickel (Ni) and vanadium (V).

In order to extract, from the above results the most favorable combinations of elements for yield strength improvement, we have quantified the range of the key elements among themselves: Chromium and Copper (0.1–0.5%), Manganese (1.7–0.65%), phosphorus and sulfur (0.02–0.035%) and Silicon (0.3–1.4%).

5. Discussion

There are currently numerous studies investigating the relevance of the addition of alloying chemicals in steels [36,37]. However, only a few studies have shown the influence

of the combination of these chemical elements [33,38–40]. The novelty and importance of our approach lie in being able to evaluate the influence of the combination of the alloying chemical elements, through the complex network approach, on such a relevant variable in terms of mechanical behavior as the yield strength of the material. The combination of elements is key in the development of the mechanical properties of steel. It has been demonstrated in numerous investigations that not only the percentage of chemical elements added has an influence, but also the interaction between the elements that make up the alloy, which can modify the final microstructure and, therefore, influence the mechanical properties [41–44].

In this section, we discuss the methodology applied as well as the results obtained. For this purpose, we first focus on the relationships of the elements that can have the greatest influence on the improvement of the yield strength of the steels and then on the elements whose addition can be key to the improvement of this parameter.

Within the applied methodology it has been shown that the classical betweenness centrality measure does not solve the objective of analyzing, both locally and globally, the influence of the combinations of chemical elements within the steel. In order to clarify the advantage of the application of the RRWG centrality measure versus the classical centrality measure betweenness, a summary table of results has been made (see Table 4). In this table, the rate of shared elements and the mean yield strength for the first ten structural steels of both rankings obtained are shown.

Table 4. Ranking comparison: Classic betweenness centrality (BT) vs. return random walk gravity centrality (RRWG). The first column is the 10-top material composition using both methods, the second column is the yield strength average of these materials, the third column is the ratio of the shared elements between them, and the fourth column is a similar ratio, but using only the fifth most relevance chemical elements of this kind of materials.

Method	Yield Strength (Avg)	Shared Ratio Top-10 (%)	Shared Ratio Top-5 (%)
BT	229.2	2.05	1.545
RRWG	532.8	2.851	1.984

The results of Table 4 ratify the use of the RRWG. It shows better results, not only in the mean of the fundamental parameter as it is Yield strength but also in the ratio of shared elements among the best-positioned structural steels.

Once the adopted methodology has been justified, the discussion focuses on the relationships between the elements that have proved to be beneficial for the improvement of the yield strength.

One of the most relevant combinations as shown by the results of the study is Cr-Cu. The combination of these elements, Cr and Cu, has been widely studied for their relevant role, jointly and separately, in the corrosion behavior of steels [45,46]. Numerous specific studies have demonstrated the relationship between yield strength and corrosion resistance [47,48]. Therefore, it is not surprising that both Cu and Cr and the action of the combination of both in steel can lead to an improvement in the yield strength of steels. Therefore, the good results obtained from the position occupied in the ranking by steels showing this combination of elements, Cr and Cu, in terms of their influence on the yield strength value are ratified.

It is worth highlighting the good results of the yield strength value obtained in this work for steels with combinations of chemical elements such as silicon, manganese, and phosphorus. The joint addition of manganese and silicon in steels and the influence on their microstructure and mechanical properties is known in some steel grades [33,38,39]. The combination of elements such as manganese, silicon, and phosphorus has been shown to be the cause of solid solution in high-strength enameled steel and this fact has been determined using empirical relationships between microstructure and yield strength [49]. Silicon is one of the most important elements in the material that occupies the number one position in

the ranking in relation to the rest of the steels that occupy good positions. It should also be noted that it is the element whose absence in relation to other chemical elements in the structural steels analyzed leads to a decrease in the value of the yield strength according to the results shown. It has been shown that the addition of this element affects the creep behavior of carbon steels as it affects the initiation of dynamic recrystallization, with an increase in the deformation necessary to initiate dynamic recrystallization [36]. The results obtained based on the combination of this element, Si, in the different steels ratify the great relevance that the addition and proportion of this element has on the value of the yield strength.

The steels with combinations of chemical elements such as Ni-Cr and Mo also obtained very good positions in the results analyzed. As for the combination of chemical elements such as Ni-Cr and Mo, their relevance in stainless steels is well known, presenting a wide range of mechanical properties such as, for example, these alloys present excellent ductility and toughness, even at high levels of resistance, and up to cryogenic temperatures [50].

All the combinations of chemical elements present in the results, which have been extracted from the structural steels with the best positions in the ranking, represent to a greater or lesser extent combinations that influence the final value of the steel's yield strength. Moreover, as we have been able to analyze the contrasted results, there is evidence of these influences. Once the most influential combinations of chemical elements on the value of the yield strength have been analysed, they can not only serve as a roadmap to create steels with better values of this mechanical parameter, but also to improve the existing ones and even apply this knowledge to improve the mix of recycled steels in the increasingly important circular economy of steel.

6. Conclusions

The influence of the combination of the chemical elements that make up the structural steels has been studied through the application of centrality measures, the most relevant conclusions being as follows:

(i) The combinations of the elements carbon-manganese-phosphorus-sulphur and silicon are determinant in the final value of the yield strength in these steels.
(ii) The combination of the chemical elements chromium and copper with the previous elements seems to have a clear influence on the increase of yield strength and should be taken into account in future experimental studies.
(iii) In addition to the above elements, the combination of these with molybdenum, nickel, and vanadium does not show strong evidence of influencing the final value of the yield strength but these should also be considered in experimental studies.
(iv) Silicon is the chemical element whose combination, with other relevant elements described, has the greatest influence on the yield strength of the structural steels analysed. The absence of this chemical element in the steel composition has a clear influence on the decrease of the yield strength.

As future work, we are investigating the incorporation, in the benchmark, of new centrality measures specific to weighted networks.

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