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RCMOS – Multidisciplinary Scientific Journal The Knowledge.
ISSN: 2675-9128. São Paulo-SP.

Year VII, v.1 2026 | Submission: April 17, 2026 | Accepted: April 20, 2026 | Publication: April 22, 2026

Supramolecular structure of cellulose and nanocrystals: a literature review

Supramolecular Structure of Cellulose and Nanocrystals: A Literature Review

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Summary:

Chemical knowledge of the structure of this carbohydrate is of paramount importance for a better understanding of its characteristics, such as hydrophilicity, chirality, biodegradability, and functionalization. The cellulose molecule is synthesized by the multimeric transmembrane cellulose synthase complex (CESA) on the surface of the plasmalemma of plant cells. Susceptible to the formation of many hydrogen bonds with each other, which leads to their crystallization into rigid, insoluble rods, the cellulose chains join together,
forming cellulose microfibrils, whose basic unit is the monomer of the monosaccharide D-glucopyranose. Depending on the production process used and the treatment applied, cellulose can exhibit distinct crystalline structures and, therefore, is
Cellulose is considered a polymorphic material. These cellulose polymorphisms are well known, the main ones being: cellulose I, II, III1, IV1 and IV1. As a consequence of the different conformations that the hydroxymethyl group can assume, two possible packing structures of cellulose chains in a microcrystal are noted: the parallel chain and the antiparallel chain, characteristic of cellulose I and cellulose II, respectively.
Currently, CNCs are obtained by different methods, including enzymatic hydrolysis, ultrasound-assisted hydrolysis, dissolution in N,N-Dimethylacetamide (DMAc)/LiCl and
in ionic liquids. However, the most commonly used methodology is acid hydrolysis. Finally, the morphology, dimensions, and properties of nanocrystals strongly depend on reaction conditions, such as time, temperature, concentration, and type of acid, and will be discussed in this literature review in order to understand the distinctions between cellulose and nanocellulose, according to their different physicochemical characteristics.
Keywords: Cellulose, Cellulose nanocrystals, Molecular structure

Abstract:

Cellulose structure, a type of carbohydrate, presents great importance for a deeper understanding of its characteristics, such as hydrophilicity, chirality, biodegradability, and functionalization. The cellulose molecule is synthesized by the multimeric transmembrane complex, cellulose synthase (CESA), on the plant cell plasmalemma. Cellulose chains form numerous hydrogen bonds with one another, leading to their crystallization into rigid, insoluble rods and amorphous regions via the D-glucopyranose monomer. Depending on the specific extraction process employed and/or the subsequent treatment it receives, cellulose may exhibit different crystalline structures; it is therefore considered a polymorphic material. These cellulose polymorphs are well-established, with the primary forms being Cellulose I, II, III, and IV. As a consequence of the various conformations, two popular cellulose polymorphs, within a cellulose microcrystal: a parallel-chain structure and an antiparallel-chain structure, are characteristic of Cellulose I and Cellulose II, respectively. Currently, CNCs, a type of nanocellulose, are obtained by various methods, including enzymatic hydrolysis, ultrasound-assisted hydrolysis, and dissolution in N, N-dimethylacetamide (DMAc)/LiCl or in ionic liquids. However, acid hydrolysis remains the most widely used methodology. Finally, the morphology, dimensions, and properties of these nanocrystals are heavily dependent on reaction conditions such as time, temperature,

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, and the specific type of acid used, and these factors will also be discussed in this literature review to elucidate the distinctions between cellulose and nanocellulose concentration based on their differing physicochemical characteristics.

Keywords: Cellulose, Nanocrystals, Molecular structure

1. Introduction

The generation of increasingly diversified products produced by the system Industrialization made the abundance of consumer goods a symbol of successful economies. modern capitalists. Alongside this context, society began to worry with sustainability issues, in order to achieve an environmental balance between industrial production and the impacts generated by its processes and products (PINTO, 2013). Thus, a new way of thinking emerged that sought sustainable solutions for development. new industrial technological alternatives and new raw materials, in order to replace the then used in order to maintain or improve the performance of end products. distinctive.

The increasing development of new technologies and the search for new sources of Raw materials for industrial use have notably provided unprecedented advances. as previously expected. Brazil now occupies the fourth position among the largest producers of cellulose is the world's largest cellulose source (BRACELPA, 2013), a material widely used in various industrial sectors.

Cellulose is the most abundant natural polymer on the planet, and it is biodegradable and... Non-toxic. A chemical understanding of the structure of this carbohydrate is of paramount importance. for a better understanding of its characteristics, such as hydrophilicity, chirality, biodegradability and functionalization.

Due to its potential as a renewable material, it has been studied for over... 150 years, with a primary focus on its biological and chemical properties. Currently, the The main focus is on its physical and mechanical properties, geared towards a variety of... end applications (COFFEY, BELL & HENDERSON, 2006).

According to Moon et al. (2011), the demands of modern society for products The differentiated and technological needs would not be met by the traditional materials used. in manufacturing processes. Sophisticated products with differentiated properties will be largely demanded by future generations, with aesthetic improvements and more vibrant colors. striking, different technological features, greater durability and, above all, greater sustainability.

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New products derived from lignocellulosic sources are being investigated, with excellent prospects for a new market, and, in this scenario, biopolymers such as Cellulose is gaining prominence as a replacement for non-renewable materials. Among the Among the known and used nanomaterials, nanocelluloses stand out, which can be... obtained through different processes, in varying sizes.

Nanotechnology and the study of nanomaterials provide, every day, valuable discoveries, not only for the development of new products, but also for a more efficient and intelligent exploitation of resources: today, there are countless sectors that employ products and byproducts on a nanometric scale.

Nanomaterials are made up of particles with at least one dimension. less than or equal to 100 nm. Cellulose nanocrystals (CNCs) are crystals obtained from from the crystalline region of the cellulose chain and are the subject of arduous studies to expand their knowledge, which opens up positive prospects for its application as a new biopolymer. industrial. Silva and D'Almeida (2009) emphasize that the great interest in studies of this The material is valued for its applicability as a reinforcing material in polymer matrices. which gives products more desirable physical properties: rigidity and flexibility. Peng et al. (2011) also cite efforts made for surface chemical modification. of the NCC, in order to achieve its potential properties.

2. LITERATURE REVIEW

2.1 Cellulose

Wood is a material used for numerous purposes, and its applications are... various, both in their natural state, in the areas of civil construction, furniture and boat manufacturing, as well as post-processed, in the manufacture of ropes, fabrics, yarns and paper (EICHHORN et al., 2010).

According to Lewin and Goldstein (1991), the chemical composition of wood presents, On average, 40 to 45% cellulose; 20 to 30% hemicellulose; and 18 to 25% lignin. broadleaf trees and 25 to 35% conifers; 3 to 8% extractives; and 0.4% ash.

Habibi, Lucia and Rojas (2010) report that cellulose is the most organic polymer. The most abundant resource on the planet, with an estimated production of more than 7.5 × 10^10 tons per year. being present in the structure of plants, in a large part of marine animals, in Algae, fungi, bacteria, invertebrate animals, and even protozoa. Brazil

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Brazil stands out in the world ranking of pulp production. According to the Brazilian Association

According to the Brazilian Pulp and Paper Association (2013), we are the 4th largest producer of pulp in the world, with

Production reached 13,922 thousand tons in 2011, representing almost 8% of total production.

worldwide during that period.

Cellulose, the main component of the cell wall (Figure 1), is a

A high molar mass polysaccharide, which presents itself as a linear chain polymer.

composed exclusively of ÿ-D-glucopyranose units linked by bonds of the type

(1-4) (FENGEL et al., 1989).

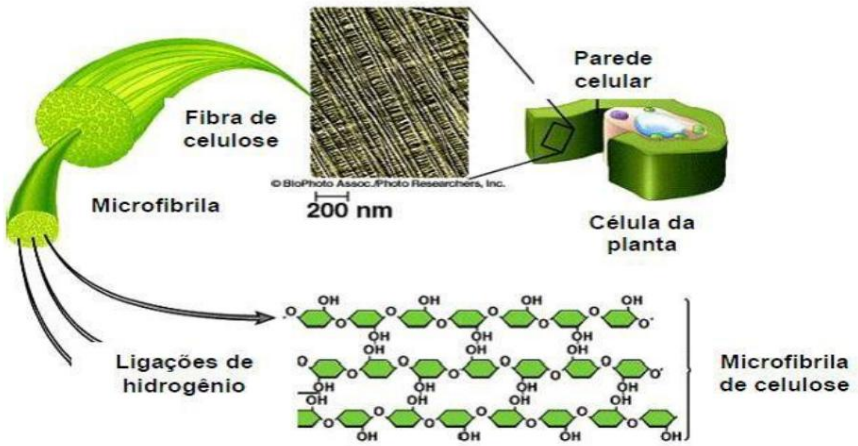

Figure 1 – Morphological structure and organization of cellulose in the cell wall.

Adapted from Doors sliding – MacGraw-Hill Companies (2012).

The cellulose molecule is synthesized by the transmembrane multimeric complex.

cellulose synthase (CESA), forming a six-lobed structure, called a rosette, in

surface of the plasmalemma of plant cells. This rosette was clearly observed by

electron microscopy (KIMURA et al., 1999), and it is believed that each rosette synthesizes

36 cellulose molecules simultaneously.

Parallel cellulose chains are susceptible to the formation of many bonds.

hydrogen bonds with each other, leading to crystallization into rigid, insoluble rods, the

Cellulose microfibrils. The elongation of cellulose molecules can occur through the movement of CESA

complexes in the plasma membrane (DÉJARDIN et al.,

2010).

The hydrogen bonds formed by the -OH groups of cellulose molecules

They can be intramolecular or intermolecular, and it is these bonds that give the structure its structure.

Cellulose's stability makes it valued as a reinforcement in composites.

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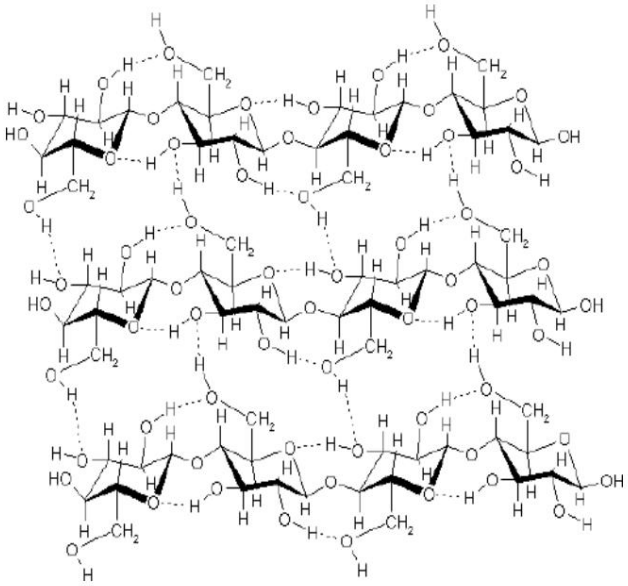

Figure 2: Intra- and intermolecular hydrogen bonds in the cellulose chain.

Source: Marabezi, 2009.

According to Moreira (2009), intramolecular bonds are responsible for The rigidity of the cellulose chain. These aggregated intermolecular bonds form microfibrils, which in turn aggregate to form fibrils, which, when ordered, These constitute the cell walls of plants. In other words, the intermolecular bonds are responsible for the formation of plant fiber.

2.2 Molecular Structure of Cellulose

Cellulose is a linear homopolymer whose basic unit is the monosaccharide. D-glucopyranose.

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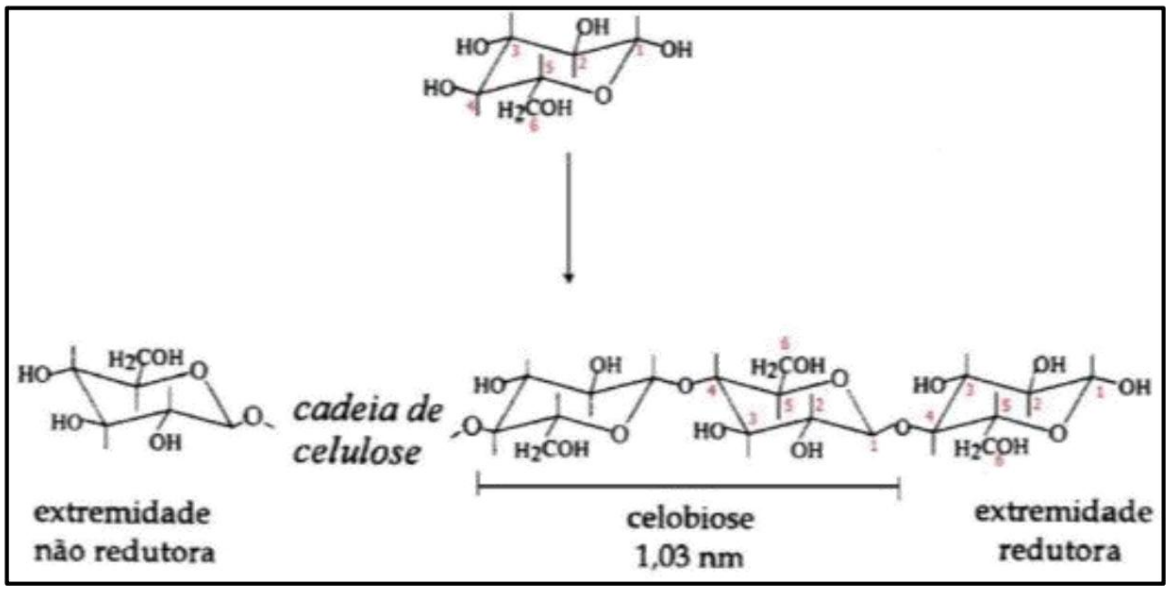

Figure 3 – Molecular structure of cellulose Klem et al., 1998.

Each anhydrous glucose unit (UAG) has two secondary hydroxyl groups attached.
to carbons C-2 and C-3 and a primary hydroxyl group attached to carbon C-6. D-glucose can
to present diverse conformations and, specifically in the case of cellulose, two
Chair conformations are possible (Figure 4). The 4C1 conformation is the most likely.
for cellulose, since the bulky groups (-CH2OH) are located in the position
equatorial, this conformation being more stable than the axial one (Daniel, 1985).

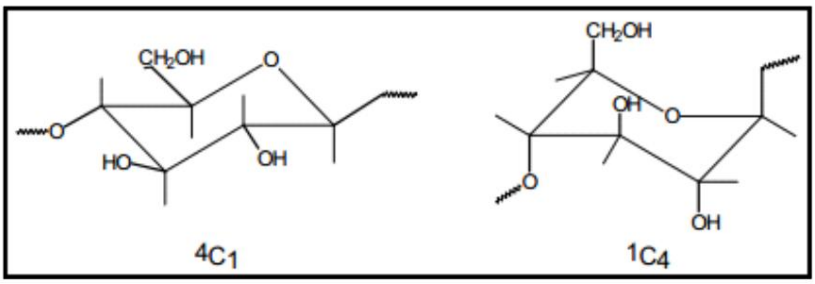

Figure 4 - Conformers for AUG in cellulose (Daniel, 1985).

The condensation of two molecules results in a mixture of macromolecules of
Various sizes; the GP of cellulose corresponds to an average value.

2.3 Crystalline Structure of Cellulose

Cellulose is a semi-crystalline polymer, meaning it has crystalline regions.
highly organized and amorphous regions, in which the chains are grouped together

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more irregular manner (French, 1985; Marchessault and Sudararajan, 1983).

The presence of hydroxyl groups in UAG generates strong hydrogen bonds. intermolecular and intramolecular forces along the polymer chain. In Figure 6 below, These bonds are represented: OH(6)---OH(3ÿ) and OH(3)---OH(5ÿ), bonds intermolecular and intramolecular, respectively.

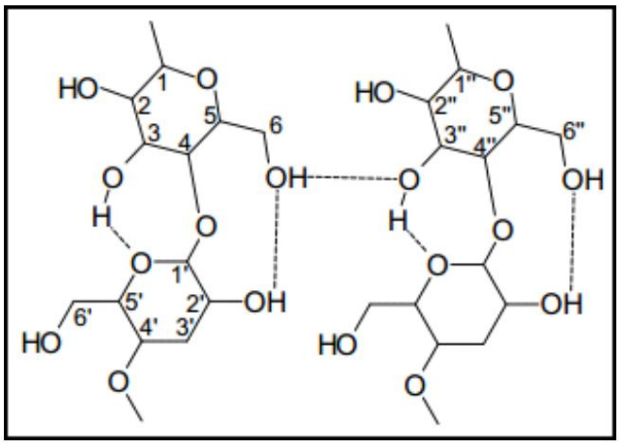

Figure 6 - Representation of inter- and intramolecular bonds in cellulose chains (Morgenstern and Kammer, 1996).

These bonds are responsible for certain properties of cellulose, because They provide high rigidity to the structure and offer a high degree of organization. crystalline (Sjöholm et al., 2000). For example, although each UAG contains three OH groups, Cellulose only swells, but does not dissolve in protic solvents.

Intramolecular bonds are responsible for the rigidity of the polymer chain. while intermolecular forces lead to the formation of plant fiber (Klemm et al., 1988).

The portion of crystalline material in a polymer, including cellulose, is called the crystallinity index (Ic). The Ic influences a number of properties of Cellulose, which is a very important structural characteristic.

2.4 Supramolecular Structure of Cellulose

Depending on the nature, the pulping process employed and/or the treatment. When received, cellulose can exhibit distinct crystalline structures and, therefore, is considered a polymorphic material (Krässig, 1986). These polymorphisms of cellulose are well known, the main ones being: cellulose I, II, III1, IV1 and IV11. The treatments, schematically represented below, they induce interconversion between polymorphs (O'Sullivan, 1997).

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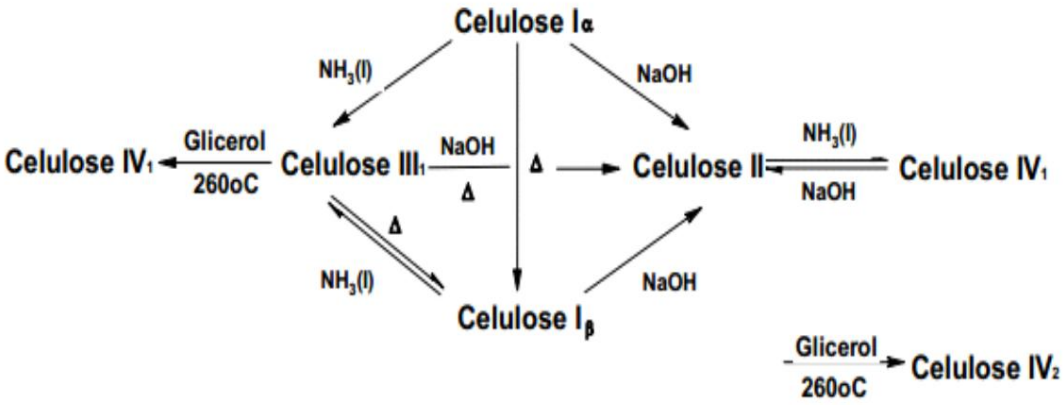
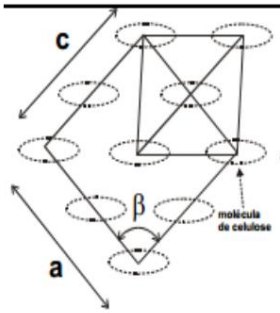


Figure 7 – Interconversion of cellulose polymers (O'Sullivan, 1997).

Each polymorph has its own crystallographic cells. Table 1 shows them. presented are the typical values of the unit dimensions observed in the shapes Polymorphic cellulose.

Table 1 - Unit dimensions of polymorphic forms (Gröbe, 1989; Klemm et al., 1988).



	Dimensões			
polimorfo	*a*, Å	*b*, Å (eixo da fibra)	*c*, Å	β (graus)
I	8,2	10,30	7,6	85
II	8,0	10,3	9,0	63
III_1	7,22-7,82	10,28	9,9	57-58
IV	8,1	10,3	7,9	90

2.5 Mercerization of Cellulose

The mercerization process was introduced industrially in 1840 and received This name is in honor of its inventor, John Mercer. In this process, the cellulose is strained in an aqueous solution of NaOH (with concentrations between 10% and 50%), with the main objective of improving the tensile strength of fibers and yarns (D'Almeida, 1988). As an example, we can cite the textile industry, in which, after the process of In mercerization, improvements are observed in cotton regarding dyeing capacity, elasticity, softness, among other properties (Rowland et al., 1984).

The purpose of the mercerization process is to convert, in a way...

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irreversible, the transformation of type I cellulose into type II cellulose, initially without degradation of biopolymer. Figure 8 shows the structures of cellulose I (native) and biopolymer. Cellulose II (mercerization product) (Gardner and Blackwell, 1975; Langan et al., 2001).

Note that the hydroxymethyl groups (-CH2OH) of cellulose I are located in The trans-gauche conformation is tg, whereas in cellulose II, this conformation is gt. The consequence of this conformational difference in the hydroxymethyl groups is that... Cellulose I exhibits an additional intramolecular linkage (HO–2' O-6) along the Chain, which does not exist in cellulose II.

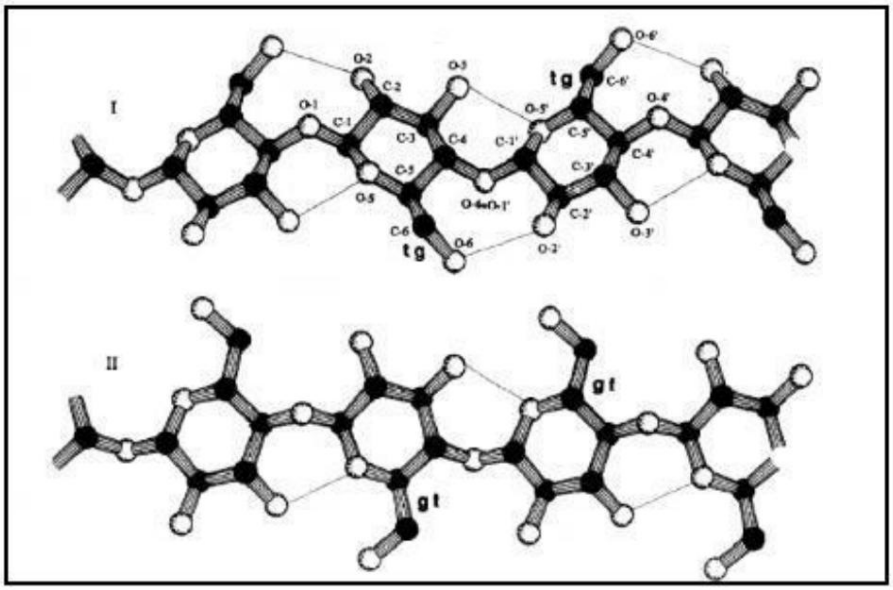

Figure 8 - Molecular models of cellulose I and II. The conformations of the hydroxymethyl groups, tg or gt, are shown. marked, as well as the indicated intramolecular bonds (Gardner and Blackwell, 1975).

As a consequence of the different conformations that the hydroxymethyl group can Assuming this, two possible packing structures of the cellulose chains can be observed. in a microcrystal: the parallel-strand and the antiparallel-strand, characteristics of Cellulose I and Cellulose II, respectively (Figure 9).

Parallel structures occur when the –CH2OH groups of adjacent chains In the antiparallel structure, these groups are on the same side, whereas in the antiparallel structure, these groups are on the same side. They meet on opposite sides of the polymer's "backbone".

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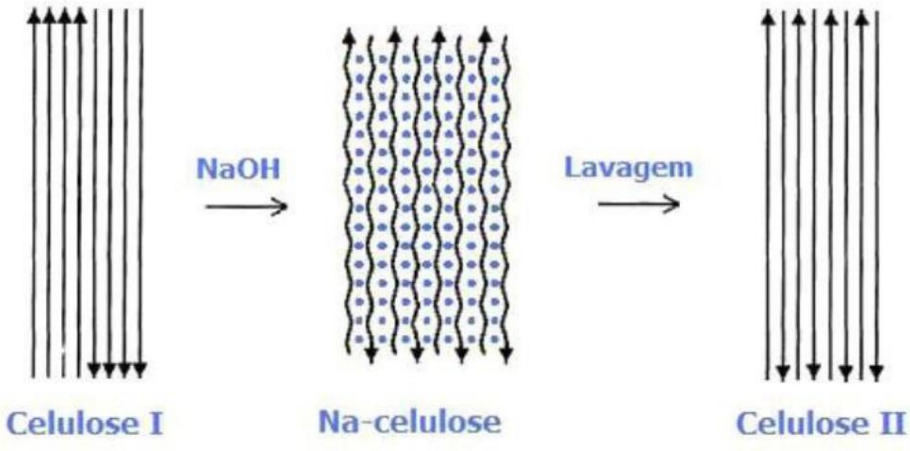

Figure 9 – Representation of Cellulose I (parallel) and Cellulose II (antiparallel) chains (Kroon-Batenburg and Kroon, 1997).

Note (Figure 10) that antiparallel packing (cellulose II) allows the formation of hydrogen bonds to a greater extent along the chains, generating three-dimensional scale arrangements, resulting in a lower energy structure and, Consequently, greater stability. This structural characteristic can be a a plausible explanation for the fact that cellulose II is not converted into cellulose I (of lower density). stability) (Kroon-Batenburg and Kroon, 1997).

As a modification of the crystal structure pattern, mercerization generates: (i) an increase in the interplanar distance between cellulose chains in the crystal lattice, of 0.6 nm in cellulose I to 0.76 nm in cellulose II; and (ii) an increase in longitudinal dimension in unit cell size, from 0.79 nm in cellulose I to 0.91 nm in cellulose II (Krässig, 1996).

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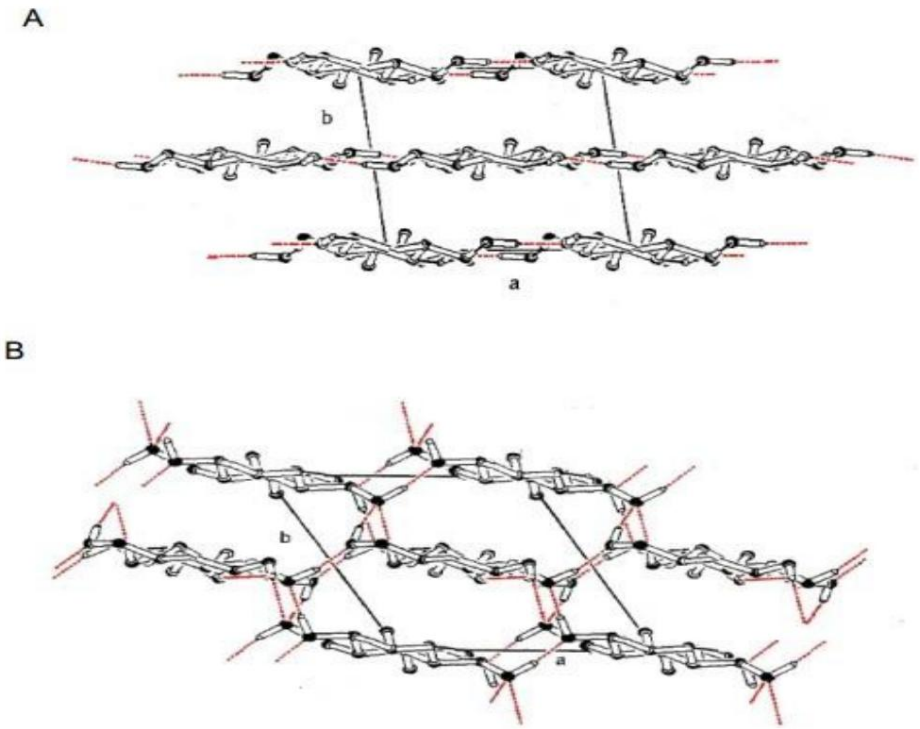

Figure 10 - Projection of the cellulose unit cell onto plane a,b. In A: representation of cellulose I (chain parallel). In B: representation of cellulose II (antiparallel chain); (---- represents the bonds of hydrogen between the chains) (Kroon-Batenburg and Kroon, 1997).

Cellulose I can be converted into cellulose II (Figure 11) by means of two Processes: regeneration and mercerization. The regeneration process involves preparation. from a solution of cellulose in a suitable solvent or in an intermediate derivative, followed by coagulation and recrystallization.

Mercerization, on the other hand, involves the swelling (intracrystalline and intracrystalline) of cellulose in concentrated NaOH solutions, followed by washing and recrystallization, as explained above.

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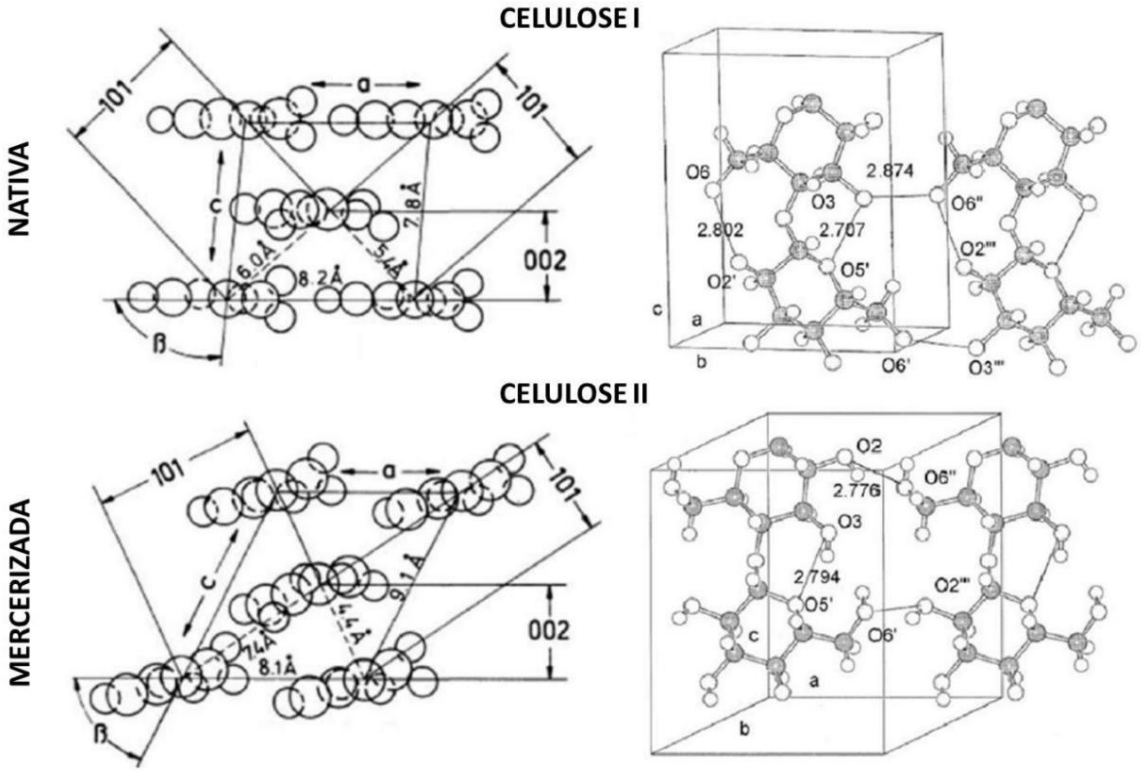

Figure 11 – Comparison between the unit cell structures of Cellulose I and Cellulose II.

2.6 Nanocellulose

Cellulose is considered a very interesting material for use as reinforcement.
at the nanometer scale, because it is obtained from a renewable and biodegradable source,
because it has a high modulus and high strength, low density and low cost.

Cellulose nanoparticles may have several names in the literature:
cellulose nanowhiskers (CNW), whiskers (Wh), cellulose nanocrystals (NCC),
Nanocrystalline cellulose (CNC), nanofibers (NF), nanocellulose, among others. (SIQUEIRA,
BRAS and DUFRESNE, 2010).

2.7 CNC Nanocrystalline Cellulose

Especially in cellulose, these crystalline domains, isolated from the
Acid hydrolysis of fibers, they are called cellulose nanocrystals (also known
such as whiskers or nanocrystalline cellulose), as shown in Figure 12. These crystals
They have axial physical properties close to those of perfect crystals (CHENG,

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DEVALLANCE, et al., 2011).

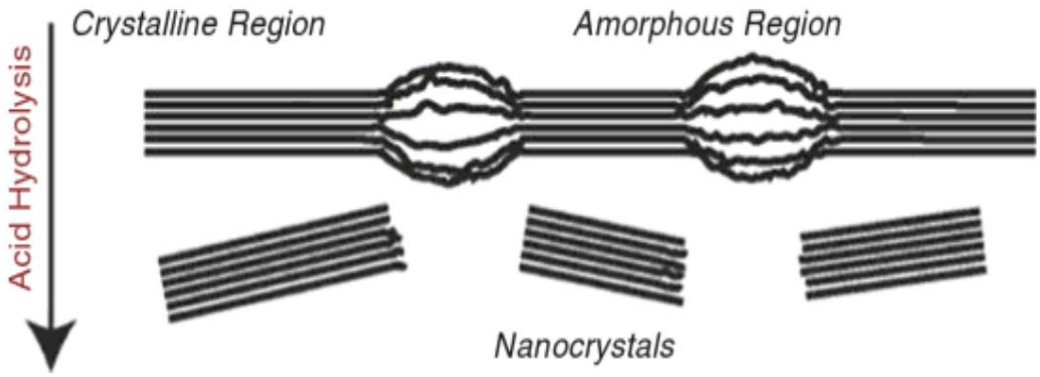

Figure 12 – Illustrated mechanism of cellulose nanocrystal formation (PÄÄKKÖ et al., 2007).

Cellulose *whiskers* can be isolated from different fiber sources.
plant-based cellulosic materials (DUFRESNE et al., 2000; LU et al., 2005; TEIXEIRA et al., 2007; CHERIAN et al., 2008), and Milewski (1994) reports that cellulose whiskers These are regions that grow under controlled conditions, which allows for the formation of crystals. High purity individuals. This highly ordered structure can confer not only high resistance, but also significant changes in some properties. important properties of materials, such as electrical, optical, magnetic, ferromagnetic, dielectric and conductivity properties.

The tensile strength properties exhibited by these nanocrystals are far superior to those of other materials with a high surface-to-volume ratio, which allows the processing of composites with improvements in their intrinsic properties (SAMMIR, ALLOIN and DUFRESNE, 2005).

Cellulose nanocrystals have several advantages compared to other materials. Nanomaterials, for example, have advantages such as ease of formation and low cost. from the raw material, the diverse characteristics depending on the natural substrate of origin and also mechanical properties, compared to those of carbon nanotubes and inorganic nanofibers (SILVA et al., 2009).

2.8 CNC Production

The most commonly used method for obtaining cellulose nanocrystals is hydrolysis. with strong acid, through which nanocrystals are obtained, generally with a size of 100-200 nm.

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of length and 20-40 nm in width, as reported by Cao et al. (2010). It can-
It is said that the amorphous region in cellulose is more easily accessible to acid and more susceptible to hydrolytic action rather than crystalline domains. The attack of strong acid on the fibers of Cellulose formation occurs primarily in the amorphous regions of cellulose because, in addition to Because they have lower density compared to crystalline regions, they are more easily accessible. (Figure 13).

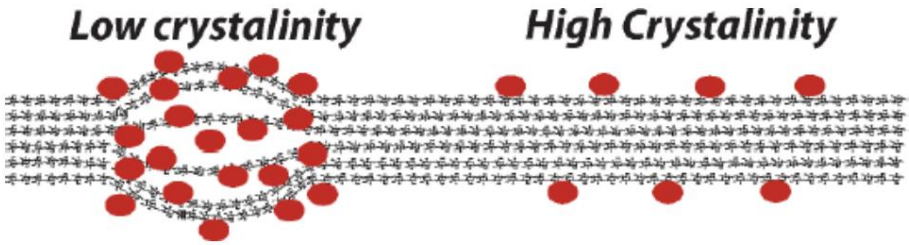

Figure 13 – Hydrolysis-promoting agents (in red); crystalline regions show lower levels of hydrolysis. attack regions, as opposed to amorphous regions. Adapted from Oke (2010).

The process of isolating nanocrystals begins with the pretreatment of Raw material, where the material is classified and, when necessary, purified. Subsequently, acid hydrolysis takes place, a step in which the crystalline domains are... preserved. Acid hydrolysis, with strong acids (such as sulfuric acid and acid hydrochloric acid (Hydrochloric acid) is currently the most widely used method for obtaining nanocrystals of cellulose. After this step, the suspension is washed by centrifugation and dialyzed. until neutrality, to the dispersion of the cellulose whiskers and to the filtration of the suspension (SILVA and D'ALMEIDA, 2009).

Various acid hydrolysis conditions have been studied to assess the nature physics and chemistry of the cellulose nanocrystals obtained. Among these various methodologies, The use of sulfuric acid (H2SO4) has been highlighted in the condition studied by Sonesso. (2011), in which esterification of hydroxyl groups by sulfate ions occurs during the hydrolysis stage. This fact causes the nanocrystals to exhibit a surface charge. Negative. This anionic stabilization, resulting from the attractive/repulsive forces of the double bond. The electrical layer is probably the reason for the stability of the colloidal suspension of nanocrystals, according to Lu et al. (2010), cited by Kargarzadeh et al. (2012).

Habibi, Lucia and Rojas (2010) further emphasize that phosphoric acid and acid Hydrobromic acids can also be used in acid hydrolysis, although on a smaller scale. According to Elazzouzi-Hafraoui et al. (2007), when sulfuric acid is used in

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ISSN: 2675-9128. São Paulo-SP.

Year VII, v.1 2026 | Submission: April 17, 2026 | Accepted: April 20, 2026 | Publication: April 22, 2026

In acid hydrolysis, the CNC obtained disperses more rapidly in aqueous medium than the obtained with hydrochloric acid. In the second hydrolysis, it was observed that their dispersions They tend to flocculate. Furthermore, there are differences in thermal and rheological behavior. among the nanocrystals obtained. Araki et al. (1998) report that hydrolysis with acid Sulfuric acid resulted in more stable nanocrystals in suspension due to the high charge. Negative energy generated by sulfate groups present on the surfaces of the crystallites, resulting from the esterification of hydroxyl groups.

2.9 Nanocrystals: Surface and reactivity sites

Currently, CNCs are obtained through different methods, including hydrolysis. enzymatic, ultrasound-assisted hydrolysis, dissolution in N,N-Dimethylacetamide (DMAc)/LiCl and in ionic liquids. However, the most commonly used methodology is hydrolysis. acidic. During the reaction, the amorphous regions, which are more accessible, are attacked more quickly. faster than crystalline domains, which remain intact after the process. conducted in a controlled manner.

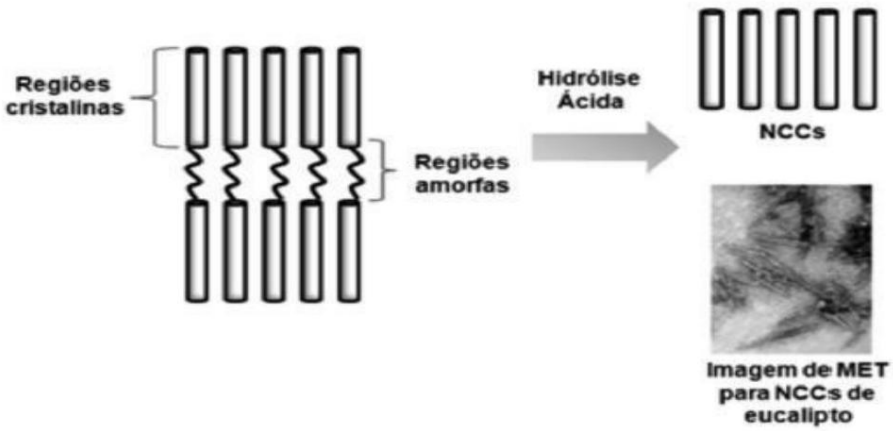

Figure 14 – Obtaining CNCs. Adapted from Pereira et al. (2014).

The typical procedure for obtaining nanocrystals (Figure 15), or *nanowhiskers* The process of dispersing cellulose in aqueous solution involves subjecting the cellulosic fibers to hydrolysis. acidic (H_2SO_4 or HCl) under controlled time and temperature conditions.

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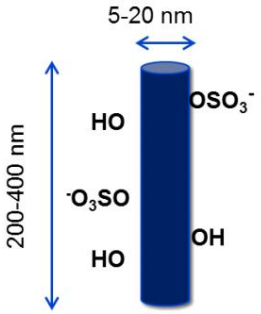

Figure 15 – Representative diagram of the physical structure of CNC (by the authors).

The morphology, dimensions, and properties of nanocrystals depend strongly dependent on reaction conditions, such as time, temperature, concentration, and type of acid. When hydrochloric acid is used, a material with limited dispersion is obtained. in aqueous solution, since the particles tend to clump together due to the high probability of hydrogen bond formation. On the other hand, when it is used In addition to hydrolysis, a direct reaction occurs between the acid and the hydroxyl groups in H2SO4. forming negatively charged ester-sulfate groups, as shown in Figure 16. The presence of these charges on the surface of the nanocrystals generates electrostatic repulsion between them. nanoparticles, which facilitates dispersion in water. On the other hand, the presence of these groups Applying the coating on the surface of CNCs reduces the thermal stability of nanostructures.

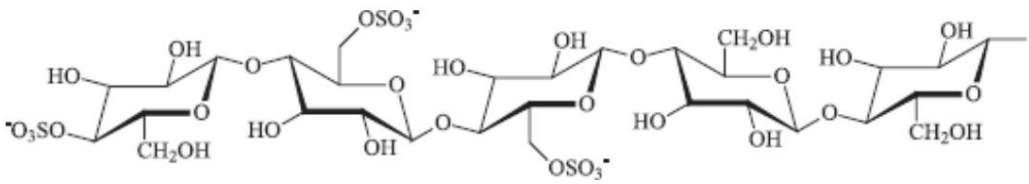

Figure 16 - Sulfate ester groups introduced into cellulose chains during CNC preparation with H2SO4. Adapted from Pereira et al. (2014).

In this way, the very process of obtaining cellulose nanocrystals can to be characterized as a modification process at the molecular structure level and supramolecular, assumed by nanocrystals.

2.10 Functionalization and surface modifications in nanocrystals

There are some obstacles to the application of cellulose nanocrystals such as nanoreinforcement, such as the prolonged time required for its production and the low cost, is a drawback.

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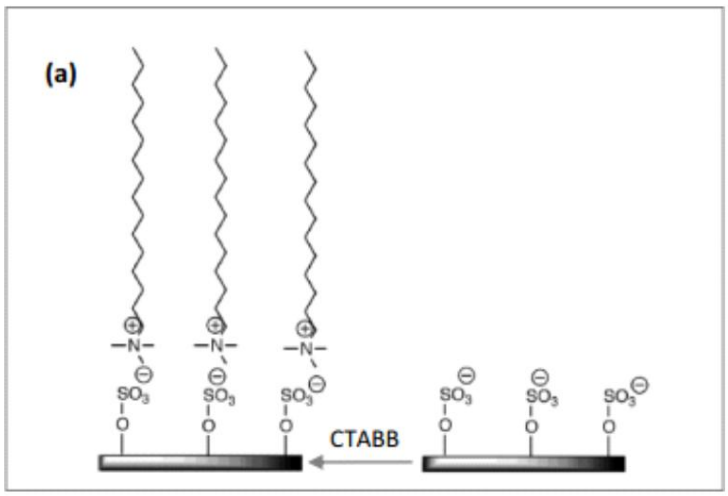
yield. Furthermore, due to the presence of hydroxyl groups in its structure, the Cellulose has a predominantly hydrophilic character, which limits its application to... water-soluble polymers. In this way, the functionalization of the surface of Cellulose nanocrystals, through modifications, allow these nanocrystals assume different supramolecular structures.

Surface modification, or functionalization, of cellulosic materials can to be divided into two main categories: (i) adsorption of the modifying agent on surface of the cellulosic material; and (ii) reaction with molecules to insert them covalently bonded to the surface of the cellulose. The method of isolating the cellulosic material. It can also be considered a form of surface modification, as in the case of Hydrolysis with sulfuric acid, since the sulfate groups bind to the surface of the cellulose, promoting its esterification. Figures 17a and 17b illustrate some Alternatives for modifying the surface of cellulosic materials.



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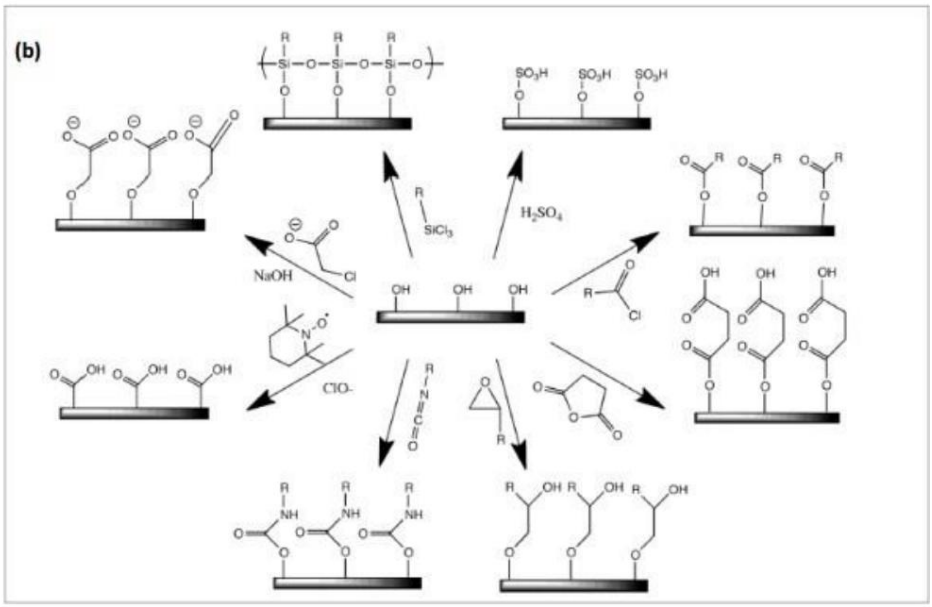

Figure 17 - Possible surface modifications of cellulosic materials: (a) by adsorption of bromide cetyltetramethylammonium (CTAB) on the surface of the cellulosic material and (b) through covalent bonding, in Clockwise: esterification with sulfuric acid, esterification with carboxylic acid halide, esterification with acid anhydride, etherification with epoxide, urethane formation with cyanates, carboxylation with N-oxyl tetramethylpiperidine (TEMPO), carboxymethylation with halogenated acetic acid, silanization with chlorosilanes.

For the chemical functionalization of CNCs, modification and the stabilization of their surfaces, with the introduction of positive electrostatic charges or negative, depending on the applications.

Zeta potential is an important physical parameter used to quantify magnitude of the electric charges of the dispersed particles and their stability in suspension, considering the solid/liquid and liquid/gas interfaces. These values can vary according to the properties of the solid/liquid interface; in the case of NCCs in a medium aqueous, which is being considered. Therefore, the surface modification of the NCC affects the distribution of ions around the interface region, increasing the concentration of counter-ions, making this interface/boundary more susceptible to diverse uses (SALOPEK, (KRASIc and FILIPOVIC, 1992)

Modifying the surfaces of NCCs is necessary so that, in addition to promoting better dispersion of the material in an aqueous medium, making its use more compatible, especially when arranged in hydrophobic or nonpolar matrices in nanocomposites (HABIBI, LUCIA and ROJAS, 2010).

Alternatively, Kalia, Kaith and Kaur (2009) state that the modification of

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NCC surfaces are essential for developing composites with superior properties.
mechanical strength, hydrophobicity, and the interface between the nanofibrils and the matrix
polymeric, promoting a larger adhesion area. For this, pretreatments are
used as an alternative to keep the surface of NCCs free of substances.
unwanted factors that could compromise the material's performance, as well as its...
Surface chemical modification and to increase the surface roughness potential.

The surface of NCCs is characterized by an abundance of hydroxyl groups, and
Various chemical modifications are emerging as alternatives to replace these.
groups by other groups (HABIBI, LUCIA and ROJAS, 2010). Among the techniques of
In the modification of the surface of natural fibers, the silylation methods stand out.
mercerization, peroxidation, benzoylation, graft copolymerization and treatment with
bacterial cellulose (silylation, mercerization, peroxide, benzoylation, graft
copolymerization, and bacterial cellulose treatment) (KALIA et al., 2011).

2.11 Organization of cellulose nanocrystals in solution

When sulfuric acid is used as a hydrolysis agent, the presence of
The sulfate groups promote a perfectly uniform dispersion of these groups. Thus, the
crystallites tend to organize themselves in a way that minimizes electrostatic repulsions (Figure
18), and concentrated suspensions tend to self-organize into crystalline arrangements,
A phenomenon similar to that observed in non-flocculating suspensions.

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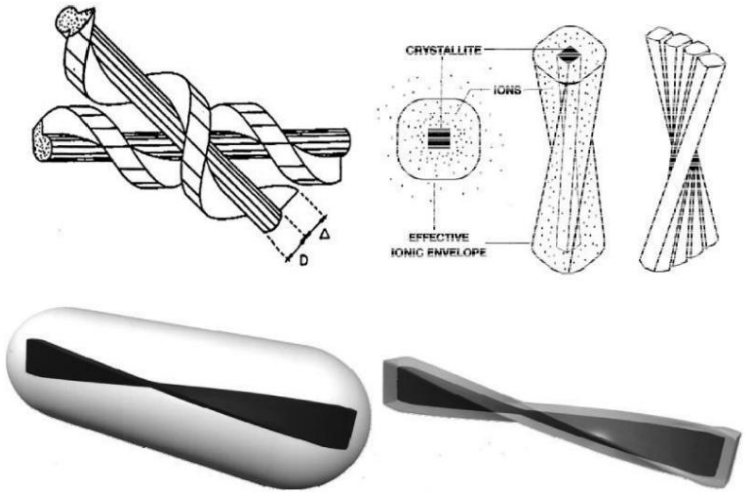

Figure 18 – Ionic envelope formed around the nanocrystal due to hydrolysis residues.
acidic, which influence the movement of the nanocrystal in the liquid medium. Adapted from Habibi et al. (2009).

According to Habibi et al. (2009), this phenomenon of self-organization was revealed due to the emergence of "fingerprint" patterns obtained from suspensions concentrated systems containing nanocrystals. Research into these systems reveals that... CNCs are randomly oriented in the dilute regime (isotropic phase). The alignment Liquid-crystalline nematic is adopted when the concentration of CNCs is high, because These nanoparticles coalesce, forming an anisotropic phase. When the suspension when a critical concentration of CNCs is reached, an ordered chiral nematic phase occurs, which It displays lines, the signature of liquid crystals (Figure 19).

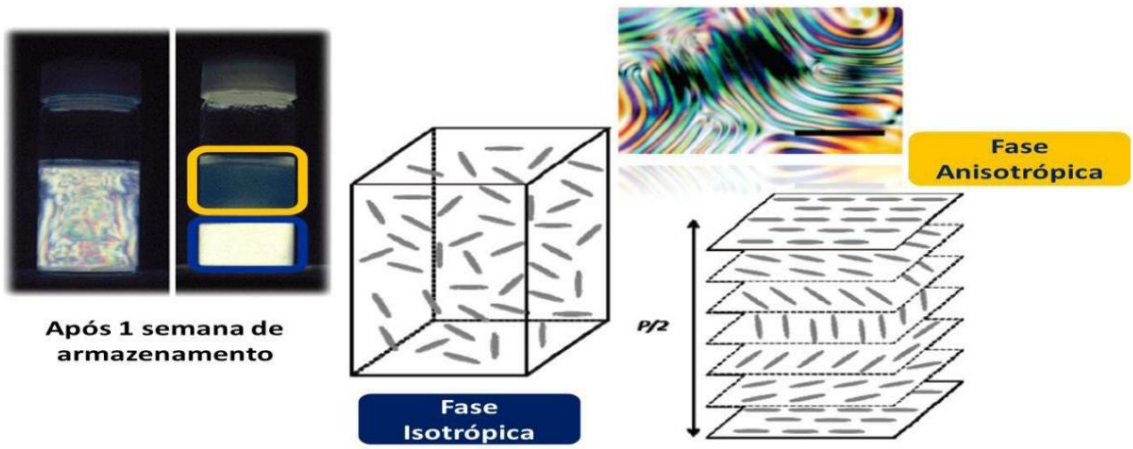

Figure 19 – Diagram of the self-organization of cellulose nanocrystals in aqueous solutions. Adapted from Habibi et al. (2009).

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2.12 Applications of Nanocellulose

Nanocellulose is considered the new biomaterial of today, mainly because it combines... due to its characteristics as abundant biological material, its physical and mechanical properties positive. The study of this new cutting-edge material has enabled its application in various areas of Structural composition of composites and nanocomposites.

In nanotechnology, the use and production of cellulose nanofibrils and their applications in Composite materials have attracted the attention of researchers because they offer high strength and stiffness combined with low weight (SIRÓ and PLACKETT, 2010).
In this way, cellulose stands out for its potential for utilizing the cellulose microfibrils present. in the cell wall of the fiber.

Composites are materials made up of a reinforcement or filler dispersed within a matrix. Therefore, it is a material formed by joining two or more materials, in which...
They take advantage of the main properties of each. Therefore, vegetable fiber acts as a reinforcement in The chosen polymer matrix. Wood is a natural example of a composite, in which cellulose acts. as reinforcement and lignin as matrix (LEÃO, 1997).

Nanocomposites constitute a new class of composites, in which at least one of the Its components have dimensions on the nanometer scale, that is, with at least one with dimensions smaller than 100 nanometers, and exhibit significantly better properties and Key differentiators. Cellulose is considered a very interesting material for use as reinforcement in nanoscale, and the study of cellulose nanofibers as reinforcement in nanocomposites. It started 15 years ago (FAVIER, 1995).

The difference between the properties of a composite and those of a nanocomposite, both produced with the same types of materials, the difference can be explained by the larger surface area of the nanocomposites, which allows for greater interaction between the nanoparticles and the matrix in which they are located. inserted (ASSIS et al., 2012).

The degree of adhesion between the fiber and the matrix is one of the main requirements for the construction of a resistant composite (LEÃO et al., 2005). Several industrial sectors have been developing Products based on composites reinforced with natural fibers in polymer matrices. especially in civil construction, the automotive industry, and the packaging industry.

Different applications of composites reinforced with lignocellulosic materials are listed by LEÃO et al. (2005): geotextiles, filters, absorbents/adsorbents, composites. Structural, non-structural composites, molded products, packaging and combinations with others materials.

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Biodegradable polymers have some limitations that prevent them from replacing...
plastics are completely affected, such as the narrow processability window (due to their temperature).
casting), thermal degradation, brittleness, and high cost. Therefore, obtaining
Bionanocomposites are a possible way to improve the properties of biodegradable polymers.
In this case, the composites can be bioplastics or biomaterials (SANTOS, 2010).

Countries such as Japan and the United States (USA) are currently the leaders in the production of
Composites made from plant fibers. In the last decade, the production of these products has increased.
exponentially. In Germany, 19,000 tons of natural fibers were used in 2005.
in automotive composites, excluding wood and cotton, according to KARUS and GAHLE
(2006).

The use of nanocomposites by automakers in the US could save 1.5
billions of liters of gasoline in a year and, consequently, reduce CO2 emissions by more than 7.5 million tons,
due to the intrinsic characteristics of nanofibrillar cellulose (LEÃO et al.)
al., 2005).

The potential for natural fiber in Brazil today is around 40,000 tons/year for industry alone.
automotive — approximately 20 kg/car of natural fibers —, not counting new markets, such as
civil construction and electronics (SANTOS, 2010). Therefore, cellulose nanofibers, by
exhibiting a high elastic modulus, they constitute a strong alternative for improving
properties in the production of nanocomposites.

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ACKNOWLEDGEMENTS

The authors express their gratitude to the Federal University of Viçosa and to Professor Emeritus Jorge Luiz. Colodette.

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