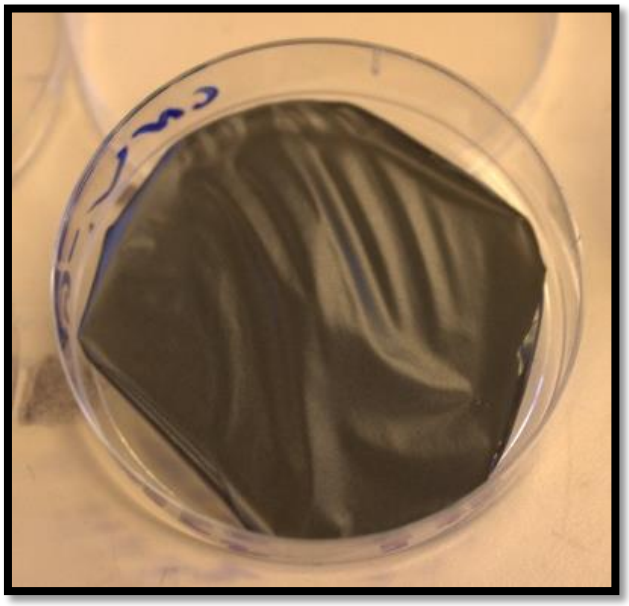


Influence of Graphene Oxide and Molybdenum Disulfide on the Structural Integrity and Physical properties of CNC Films

Bachelor's thesis in Chemical Engineering

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DEPARTMENT OF CHEMISTRY AND CHEMICAL ENGINEERING

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Gothenburg, Sweden 2026
www.chalmers.se

CHEMICAL ENGINEERING BACHELOR´S THESIS 2026

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Chemical engineering project report 2026

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Cover: Image of a CNC based film with molybdenum disulfide and Graphene Oxide additives

Gothenburg, Sweden 2026

Sammanfattning

I takt med att efterfrågan på hållbara och kostnadseffektiva funktionella material ökar, har integreringen av förnybara strukturella baser och högpresterande tillsatser blivit ett centralt forskningsområde. Denna tes undersöker syntes och karaktärisering av kompositfilmer med kristallin nano cellulosa (CNC) som strukturell bas, förstärkt med Grafenoxid (GO) och molybdendisulfid (MoS_2). Kompositerna syntetiserades via sonikering och centrifugering, följt av avdunstning på polystyrensubstrat.

Inledande försök identifierade vikten av en lägsta CNC-koncentration för att etablera ett vätebundet nätverk starkt nog att motstå kapillarkrafter under torkningsprocessen. Optimerade filmer framställdes därefter med volymförhållandena 1:1 och 3:1 (CNC-lösning till stamlösning). Karaktäriseringen uppvisade tydliga morfologiska och optiska skillnader: CNC-GO filmerna var ogenomskinliga och glansiga, medan CNC-MoS_2 filmerna uppvisade en halvgenomskinlig ”frostad” yta med hög vidhäftning mot substratet.

Nämnvärt är att det ternära systemet CNC-GO-MoS_2 vid ett 1:1 förhållande uppvisade en synergistisk effekt som resulterade i den mest robusta och flexibla filmen, med en böjningsgräns på 90^{O}. Elektrisk utvärdering visade att alla filmer förblev isolerande (> 20 MΩ), vilket sannolikt beror på sp^3-hybridiserade domäner i det oreducerade GO-materialet som stör det π-konjugerade system, som i sin tur krävs för elektrontransport. Dessa resultat ger en grundläggande förståelse för interaktioner mellan 2D material och nanocellulosamatriser och belyser potentialen hos ternära hybrider för framtida flexibla, biobaserade komponenter.

Nyckelord: CNC, GO, MoS_2, Ternär film

Abstract

As the global demand for sustainable and cost-effective functional materials grows, the integration of renewable scaffolds with high-performing additives has become a critical research avenue. This thesis investigates the synthesis and characterization of composite films utilizing Crystalline Nanocellulose (CNC) as a structural base, reinforced with Graphene Oxide (GO) and Molybdenum disulfide (MoS_2). The composites were synthesised via probe sonication and centrifugation, followed by evaporation-casting on polystyrene substrates.

Preliminary trials identified that maintaining a minimum CNC concentration is mandatory to establish a hydrogen-bonded network strong enough to withstand drying-induced capillary forces. Optimized films were subsequently produced at volumetric ratios of 1:1 and 3:1 (CNC-to-stock solution). Characterization revealed that while CNC-GO films were opaque and reflective, and CNC-MoS_2 films were semi-translucent with high substrate adhesion, the ternary CNC-GO-MoS_2 system exhibited a unique synergistic effect. At 1:1 ratio, the ternary hybrid yielded the most robust and flexible film, achieving a 90^O bending threshold, a significant improvement over the brittle binary equivalents.

Electrical evaluation confirmed that all films remained in an insulating state (>20 MΩ), attributed to the sp^3-hybridized domains within the unreduced GO which disrupt the π-conjugated system required for electron transport. These findings provide a foundational understanding of 2D material interactions within nanocellulose matrices and highlight the potential of ternary hybrids for the development of future flexible, bio-based components.

Keywords: CNC, GO, MoS_2, Ternary film

Acknowledgments

Primary, we would like to express our sincere gratitude to our examiner, Professor Gunnar Westman, for his invaluable guidance throughout this project. His expertise and feedback were instrumental in shaping the final direction of our research. Secondary, we also want to express our gratitude to Ph.D. Jelka Feldhusen for contributing valuable insights and concrete suggestions for improvement during our report writing.

Jamie Grabo & David Rogdahl, Gothenburg, March 2026

List of Acronyms

Below is a list of frequently used acronyms used throughout the work, listed in alphabetical order:

CNC – Crystalline Nanocellulose

GO – Graphene Oxide

MoS_2 – Molybdenum disulfide

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1

Introduction

1.1 Industrial & environmental demand

As modern technology and industry advance, concerns regarding the sustainability and long-term environmental impact of commercial manufacturing have become increasingly prominent [1 - 2]. Many products, ranging from plastic shopping bags and synthetic textiles to batteries, rely heavily on non-renewable and environmentally impactful materials such as petroleum and heavy metals [3 - 5]. As such, there has been a push to develop more sustainable alternatives. One of the main areas that is currently being explored is the materials chemistry [6 - 7]. Substituting conventional raw materials with less environmentally harmful alternatives that maintain or enhance the product performance offers a clear advantage for both the consumers and producers.

1.2 Current material alternatives

Extensive research has evaluated diverse material classes to mitigate these environmental impacts. In the plastics sector, Polylactic acid (PLA) has emerged as a viable bioplastic alternative to petroleum-based polymers like ABS and PET [8]. While PLA has gained widespread adoption in 3D-printing, further development is required before it can fully replace mainstream industrial plastics in other areas [9-10]. Similarly, the battery industry is seeking alternatives to conventional lithium-ion systems due to the severe environmental degradation associated with lithium mining [11 – 12]. Sodium-ion batteries represent a promising pathway forward, offering a more cost-effective and lower-impact energy storage solution utilizing abundant materials [13]. Structural engineering has also seen shifts towards sustainability; Mass timber variants, such as cross-laminated timber, are increasingly trialed as substitutes for energy-intensive structural steel due to their high load-bearing capacity and comparatively low density [14 – 15].

1.3 Cellulose and Crystalline Nanocellulose (CNC)

Amid these developments, cellulose has garnered significant research interest owing to its structural versatility and immense hydrogen-bonding potential [16 – 17]. A highly refined variant, crystalline nanocellulose (CNC), is typically isolated via acid hydrolysis to yield highly crystalline, rod-shaped nanoparticles [18 – 19]. CNCs have demonstrated utility across remarkably diverse fields, serving as a stabilizing thickening agent in low-calorie food products [20], acting as a targeted vehicle for sustained drug delivery [21], and even functioning as a lightweight component in body armour due to its needle-like structure that rivals the performance of Kevlar [22].

1.4 Advanced composites

One of the most promising applications of CNC lies in the development of polymer matrix composite materials [23]. Depending on the selection of specific filler materials combined with the CNC matrix, a diverse array of mechanical and morphological characteristics can be engineered [24]. This capacity to tailor macroscopic material properties through strategic filler selection has established CNC-based composites as a compelling research domain that offers a wide variety of industrial applications. For instance, incorporating CNCs into various plastics serves as an environmentally sustainable reinforcement that simultaneously enhances tensile strength, stiffness, and durability [25]. Additionally, CNCs can be utilized to fabricate flexible, versatile biofilms whose precise functional profiles are governed by the specific co-fillers embedded within the matrix [26].

1.5 Properties and applications of graphene oxide

A co-filler currently receiving significant attention is graphene oxide (GO), a two-dimensional layered nanomaterial derived from the controlled oxidation of graphene. This oxidation process introduces a high density of oxygen-containing functional groups, including carboxyl, hydroxyl, and carbonyl groups onto the carbon lattice [27]. The abundance of these hydrophilic groups grants GO exceptional dispersibility in aqueous systems while providing numerous active sites for secondary interactions with adjacent material phases. When coupled with its intrinsically high specific surface area, robust mechanical strength, and tuneable electrical characteristics, GO has attracted substantial interest across the fields ranging from electrochemical sensors and energy storage devices to separation membranes and structural composites [28].

Particularly advantageous synergistic properties emerge when GO is blended directly with nanocellulose matrices. Because the nanocellulose surface displays a high concentration of exposed hydroxyl-groups, strong interfacial interactions, predominantly governed by hydrogen bonding, are established between the two materials [29]. These dense interfacial networks facilitate efficient stress transfer and promote structural stability, thereby enabling the resulting binary composite to exhibit mechanical and functional performance that surpass those of either individual component.

Consequently, recent literature demonstrates that binary nanocellulose-graphene oxide (NC-GO) composites can be precisely engineered for diverse applications. Such frameworks have been investigated as high-efficiency gas sensors, where analyte interactions with the oxygenated functional groups allow for the selective detection of volatile organic compounds at room temperature [30]. They have also shown utility as water purification membranes, where GO incorporation enhances both structural stability and overall filtration throughput [31]. Furthermore, studies note marked improvements in fundamental mechanical profiles, including absolute tensile strength and fracture toughness upon embedding GO into the nanocellulose matrix [32].

While these binary investigations underscore the versatility of NC-GO frameworks, they also raise critical questions regarding whether the incorporation of additional, distinct functional fillers could achieve further performance gains.

1.6 Properties and applications of molybdenum disulfide

To complement the functional attributes of carbon-based nanomaterials, transition metal dichalcogenides (TMDCs) have emerged as highly attractive candidates for advanced composite engineering [33]. Among these, molybdenum disulfide (MoS_2) represents a prominent two-dimensional layered material characterized by a central plane of molybdenum atoms covalently sandwiched between two layers of sulphur atoms [34]. This unique atomic configuration yields exceptional intrinsic properties, including robust mechanical strength, a tuneable electronic bandgap, and high thermal stability [35]. Furthermore, the weak van der Waals interactions between adjacent MoS_2 sheets permit low-shear interlayer sliding, which renders the material highly effective for enhancing structural flexibility and dry lubrication profiles within a host matrix [36].

To successfully utilize the two-dimensional advantages of MoS_2 within polymer matrices, the bulk crystalline material must be separated into individual thin nanosheets. This transition necessitates disrupting the weak interlayer van der Waals forces that bind adjacent sheets together while preserving the strong covalent intra-layer bonds between the molybdenum and sulphur atoms [37]. There are both chemical methods, such as Chemical vapor deposition (CVD) [38], and mechanical methods, such as sonication [38]. One of the primary separation methodologies that have emerged is Liquid phase exfoliation (LPE). It is utilized due to its simplicity, scalability, and compatibility with subsequent solution processing [38]. This technique relies on external mechanical energy, typically delivered via high-intensity ultrasonication, to induce localized acoustic cavitation within a solvent medium [38]. The violent growth and subsequent collapse of the microscopic bubbles generate intense shear forces that overcome the interlayer attraction, peeling individual nanosheets away from the bulk crystal [37]. When exfoliated into thin nanosheets and integrated into polymer networks, MoS_2 can fundamentally alter a composite´s electronic, optical, and mechanical characteristics [39].

Within the context of this study, establishing a dedicated baseline for MoS_2 behaviour is important for ensuring that its specific contributions to the composite matrix can be accurately isolated and distinguished from those of other fillers. Consequently, isolated binary CNC-MoS_2 systems must be evaluated to map how systematic changes in MoS_2 loading dictate film morphology, mechanical integrity, and optical performance. Resolving these discrete baseline characteristics serves as a mandatory prerequisite to evaluating how MoS_2 behaves when co-incorporated with other distinct inorganic materials.

1.7 The knowledge gap

The promising performance of binary nanocellulose-graphene oxide and nanocellulose-molybdenum disulfide composites naturally raises the question of whether additional functional fillers can further enhance material performance. More recently, material science research has begun evaluating ternary composite systems that integrate a third functional material. Preliminary investigations indicate that the introduction of a tertiary component can yield distinct synergistic reinforcement effects, driven by the activation of multiple concurrent interfacial interaction mechanisms [24, 32]. However, while binary NC-GO and NC-MoS_2 composites have been comprehensively characterized, comparatively few studies have transitioned to examining the co-incorporation of multiple distinct functional fillers within a singular, continuous nanocellulose matrix [27, 32].

Consequently, systematic research is necessary to clarify exactly how auxiliary fillers alter composite morphology, interfacial bonding networks, and overall material performance [27, 32]. A fundamental understanding of these multi-component interactions is mandatory to definitively determine whether ternary matrices offer advantages over their traditional binary counterparts.

1.8 Aim & scope

To address the current lack of clarity surrounding multi-component, CNC-based nanocomposites, this study aims to systematically investigate the structural and physical implications of co-incorporating graphene oxide (GO) and molybdenum disulfide (MoS_2) into crystalline nanocellulose (CNC) composite thin films. Initially, independent binary systems (CNC-GO and CNC-MoS_2) are evaluated to map how systematic changes in filler concentrations dictate film morphology, optical properties, and mechanical integrity. Particular emphasis is placed on isolating and distinguishing the discrete contributions of GO and MoS_2 to the observed material properties.

Building upon the baseline established by these binary controls, this work explores the synthesis and performance profiles of ternary CNC-GO-MoS_2 composite systems. While binary cellulose formulations are well documented, few investigations have addressed the cooperative effects of embedding multiple inorganic fillers simultaneously within a nanocellulose matrix. The co-introduction of both GO and MoS_2 creates opportunities for distinct synergistic interactions, potentially unlocking performance windows and multifunctional traits unachievable by either binary variant alone.

The primary objective of this work encompasses the formulation, processing, and comprehensive characterization of both the binary and ternary composite films. Analytical focus is directed toward evaluating variances in film morphology, flexibility, optical appearance, and electrical conductivity. By executing a direct, controlled comparison between the ternary composites and their respective binary counterparts, this investigation seeks to determine if reproducible synergistic enhancements occur due to the concurrent

presence of GO and MoS_2, while elucidating the underlying mechanisms driving this behaviour.

Ultimately, this research aims to refine the current understanding of interfacial bonding and structure-property relationships in sustainable, nanocellulose-based nanocomposites. Through a detailed resolution of these molecular and physicochemical assembly mechanisms, this study intends to support the broader development of sustainable, multi-functional materials featuring highly tuneable characteristics tailored for advanced engineering applications.

2

Experimental section

This section details the experimental procedures utilized to synthesise and characterize CNC composite films. It outlines the preparation of the stock solutions, the optimization of the film-casting process, and the various stages required to achieve a homogenous CNC composite film.

The thesis investigated three distinct composites: CNC-GO, CNC-MoS_2, and CNC-GO-MoS_2. The following sections describe the iterative refinement of the synthesis, including the preliminary trials and the final protocols used for the successful casting of the analysed films.

2.1 Feedstock preparation

The primary film material used in this thesis was an aqueous suspension of CNC at a concentration of 1.2 wt.%. All materials were provided in-house at Chalmers and were utilized without further purification. Two inorganic additives were incorporated into the CNC films: Graphene Oxide (GO) with 4 - 10% edge oxidation and MoS_2. To overcome the inherent incompatibility between the hydrophobic powder and the aqueous CNC, 95 % ethanol was utilized as a dispersing agent.

2.2 Creation of stock solutions

To ensure a reproducible experiment, three primary stock solutions were prepared: CNC-GO, CNC-MoS_2, and CNC-GO-MoS_2. The preparation procedure was standardized across all three systems.

For the GO solution, 0.3 g of GO powder was added to 30 mL of CNC suspension. For calculation purposes, the density of the 1.2 wt.% CNC suspension was assumed to be 1.0 g/cm^3. To facilitate the dispersion of the hydrophobic additives, 5 mL of 95 % ethanol was added to the mixture. Regarding the other mixes, utilizing the same principle: The MoS_2 solution was prepared by adding 1.5 g of MoS_2 powder to 60 mL of CNC solution. The GO-MoS_2 mixture added 1.5 g MoS_2 powder and 0.3 g GO powder to 30 mL CNC solution.

Homogenization of the solutions was achieved using a probe sonicator at 40 % intensity (300 W, 20 kHz) of the brand and model: *Sonics, VCX750 Vibra-Cell* (750 W, 20 kHz). This specific method was chosen since the GO and MoS_2 are highly hydrophobic and required high-intensity agitation to overcome the van der Waals forces keeping them from mixing with the CNC solution. In addition, this sonication should result in a more exfoliated GO and MoS_2 with a lower sheet count via breaking up the sheets. To prevent thermal degradation or excessive evaporation, an intermittent sonication cycle was employed: 20 minutes of active sonication followed by 20 minutes of cooling, for a total duration of approximately two hours. Following sonication, the mixtures were transferred to centrifugal vials and processed

at 3600 rpm for fifteen minutes with a *Thermo Scientific, Heraeus Megafuge 40.* This was done to remove any non-dispersed additive to ensure the most stable film matrix. The resulting supernatant, containing stable and dispersed additive, was extracted and stored in sealed containers for subsequent film casting.

2.3 Synthesis of composite CNC films

For each of the three stock solutions (CNC-GO, CNC-MoS_2, and CNC-GO-MoS_2), a series of dilutions were prepared to investigate the effect of different additive concentrations on the film's properties. Three volumetric ratios of 1.2 wt.% CNC solution to stock solution were selected: 1:1, 3:1, 9:1. while maintaining a constant volume of 10 mL per sample. The three ratios were chosen to give three distinct films; high, medium, and low concentration of additive.

The mixture was prepared by weighing out each component, assuming a density of 1 g per cm^3, into clean containers and was homogenized by vigorous manual agitation to ensure a uniform distribution of the additives within the CNC solution.

To cast the films, the diluted suspension was poured into polystyrene Petri dishes (Inner diameter: 86 mm, height: 14 mm), which had been cleaned beforehand with isopropanol to remove any surface contaminants. The samples were allowed to evaporate at room temperature (22 ± 2^OC) under ambient atmospheric conditions. They were left undisturbed for 48 hours until the solvent had completely evaporated, resulting in cohesive composite films. The resulting films had their electrical conductivity and thickness measured with a *UNI-T UT131 digital multimeter* and *Mitutoyo external micrometer* (range: 0-25 mm, resolution: 0.001 mm) respectively.

2.3.1 Preliminary trials

An initial set of nine samples was prepared to test the different dilution ratios. During this stage, the stock solutions were diluted with distilled water rather than the 1.2 wt.% CNC suspension. Because of limited materials, remediation was attempted by adding 5 mL of CNC suspension to each mixture, but after allowing them to evaporate it was clear that not enough solid material was present to form a cohesive film.

Upon drying, the samples exhibited severe coiling and brittleness. The resulting fragments were unsuitable for mechanical or optical characterization. The failure to form a cohesive network suggests that a minimum CNC density is required to establish a hydrogen-bonded network strong enough to withstand capillary forces during the evaporation process. Images of the unsuccessful films are provided in figure 5 below.



Figure 1. *Picture of preliminary trial CNC-films, undried (left) and dried (right). Green; GO, Blue; MoS_2, Red; GO + MoS_2.*

2.3.2 Optimized film creation

Following the preliminary trials, the film creation process was refined to ensure a cohesive and structurally sound film. Due to the limited availability of GO powder, the experimental set was limited to two volumetric ratios, 1:1 and 3:1 (CNC suspension: Stock solution).

To achieve greater film thickness compared to the preliminary tests, smaller polystyrene dishes were used (inner diameter; 53 mm, height: 11.5 mm). These optimized parameters yielded more cohesive films, but most still exhibited some degree of brittleness, except for the 1:1 ternary film that was fairly flexible compared to the others. The films had sufficient structural integrity for performing subsequent physical and optical evaluations. These films served as the basis for the results discussed in section 4.

2.4 Characterization of physical properties

Due to the exploratory nature of this thesis combined with the available laboratory resources, the composite films were characterized using an array of qualitative and semi-quantitative methods. The following six parameters were evaluated to determine how the presence of GO and MoS_2 modified the inherent properties of the CNC matrix.

2.4.1 Electrical conductivity

Surface resistance was evaluated using a digital multimeter in a two-point probe configuration. The probes were placed approximately one centimetre apart on the surface of the films. This measurement served as a qualitative assessment of whether the additives had reached the percolation threshold for electrical conductivity at this scale or not.

2.4.2 Mechanical flexibility

The mechanical properties of the films were assessed via manual bending tests. Each film was subjected to this test to determine its “snap-point”, the maximum angle of deflection before snapping apart. Due to the high brittleness and thinness of some films, a standardized tensile strength test was not feasible; Therefore, a comparative approach was utilized to evaluate the synergistic interlocking of the combined geometries.

2.4.3 Thickness and homogeneity

Film thickness was measured using a manual micrometer with a precision of 0.001 mm. To ensure an accurate reading and account for surface variations, measurements were taken at multiple points across a small portion of the film. This measurement was used to evaluate whether the additives affected the thickness of the formed films.

2.4.4 Qualitative optical analysis

In the absence of a UV-VIS spectrophotometer and a gloss meter, optical properties were evaluated through comparative visual inspections. To assess the transparency, samples were placed over a high contrast background to visually assess the opacity levels. The reflectivity was assessed by using a "light scattering" technique. A concentrated light source was directed at the film at a fixed angle while in a dark room to observe if the films favoured reflection or diffusion of the light.

2.4.5 Macroscopic surface roughness

The surface topography was characterized via visual and tactile inspection. This assessment focused on identifying surface irregularities, such as aggregates of GO or MoS_2, that might indicate poor dispersion or interfacial failure.

3

Results and discussion

This section presents the experimental findings of the synthesised CNC composite films and evaluated them through the lens of the theoretical framework established in section 2. The analysis is categorized into qualitative morphological and optical observations, followed by a discussion of quantitative data regarding surface resistance.

By comparing 1:1 and 3:1 ratio across the binary and ternary systems, the section identifies how specific additive concentrations and the interfacial chemistry between 1D, and 2D nanomaterials dictate the resulting film morphologies, optical profiles, and mechanical behaviours. While all experimental configurations successfully formed macroscopically cohesive films, the variations in coiling, transparency, rigidity, and electrical conductivity highlight the distinct roles of the GO and MoS_2 within the CNC scaffold. A picture of the films are provided below in figure 6, individual pictures of the films are available in the following 4.x sections as figures 7 – 9.

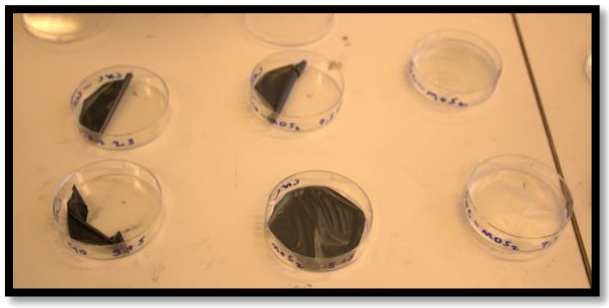


Figure 2. *Picture of optimized attempt of CNC-films, dried. From left to right; GO, GO + MoS_2, MoS_2.*

Below is table 1 that briefly shows the results of various variables of each film. A more comprehensive description of the films follows in sections 4.1 – 4.3. Most of the variables are evaluated compared to the other films on a scale of 1-6, with 1 being worst performance, and 6 being the best.

Table 1. *Summary of results*

Film/variables	**Bending angle**	**Thickness**	**Surface**	**Adhesion**
GO 1:1	4	0.061mm	Glossy	4
GO 3:1	3	0.158mm	Glossy	3
MoS_2 1:1	2	0.01mm	Frosted	2
MoS_2 3:1	1	0.005mm	Frosted	1
Ternary 1:1	6	0.009mm	Satin	6
Ternary 3:1	5	0.004mm	Satin	5

3.1 Optical profile

The optical profiles between the films provided the clearest result between the different systems. While all ratios (1:1 and 3:1) resulted in macroscopically cohesive films, the specific electron structures and geometries of the fillers created three very distinct visual profiles that could indicate the level of expression with each additive.

3.1.1 Opacity and reflectivity: The GO influence

The physical characteristics of the CNC-GO films were dominated by the presence of the Graphene Oxide nanosheets which fundamentally altered how the films interacted with light. Regardless of whether a 1:1 or 3:1 ratio was used, the resulting films produced a pitch-black, and totally opaque appearance. This total opacity is attributed to the broad absorption spectrum of the Graphene Oxide across the visible range, ensuring that even at lower concentrations, the nanosheets form a dense light-absorbing network within the CNC matrix.

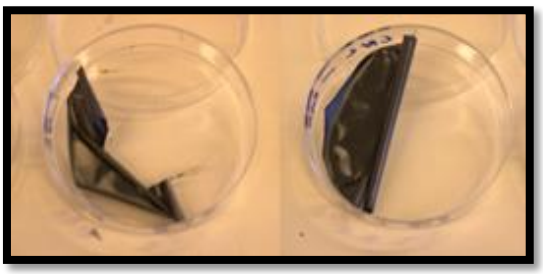


Figure 3. *Pictures of CNC-GO film (1:1) (left) and CNC-GO film (3:1) (right).*

To further evaluate the surface morphology, a “light scattering” technique was employed in a dark room using a focused light source. These evaluations revealed that the binary CNC-GO composites possessed a high degree of surface reflectivity and in turn, a glossy surface. This macroscopically smooth and reflective surface suggests a high degree of planar alignment of the GO nanosheets, creating a uniform surface that favoured specular reflection rather than diffuse scattering.

3.1.2 Translucency and substrate adhesion: The MoS_2 influence

The introduction of MoS_2 into the CNC matrix produced films with significantly different optical properties than those observed in the GO composites. At both the 1:1 and 3:1 ratio, the films exhibited a semi-translucent, matte finish comparable to that of frosted glass. This phenomenon is likely attributed to a lack of MoS_2 within the CNC matrix that can absorb or reflect the light. The more open structure of the CNC matrix probably promotes a more diffuse light scattering rather than the direct specular reflection observed in the GO composites. Combined with this unusual optical profile, closer inspection revealed the presence of small, dark surface aggregates, most likely unexfoliated MoS_2 particles that were not fully dispersed during the initial sonication process. These results suggests that some most of the MoS_2 layers exceeded the disruptive energy of the sonication probe and thus surfaced as aggregates or not at all in the CNC matrix.



Figure 4. *Pictures of CNC-MoS_2 film (1:1) (left) and CNC-MoS_2 film (3:1) (right).*

3.1.3 Ternary synergy and the "softening effect"

The ternary CNC-GO-MoS_2 films were visually a middle ground between the two binary systems, displaying a dark grey hue, a lighter gradient compared to the pitch-black CNC-GO films but still equally reflective. This shift in colour is probably the MoS_2 layers blocking the GO layers and showing their greyer colour, washing out the black of the GO layers. While small surface aggregates remained visible, the overall homogeneity of the ternary film appeared improved compared to the binary films.



Figure 5. *Pictures of CNC-GO-MoS_2 film (1:1) (left) and CNC-GO-MoS_2 film (3:1) (right).*

3.2 Mechanical integrity and interfacial synergy

The mechanical properties of the composites were evaluated through manual bending tests to identify at what angle they would snap and their overall structural resilience. These results revealed significant disparity between the binary- and the ternary films.

3.2.1 Mechanical structure of GO films

The mechanical integrity of the CNC-GO films was fundamentally governed by the interplay between the films thickness and the rigid hydrogen-bonded network within the CNC matrix. Both the 1:1 and 3:1 film exhibited noticeable coiling, a result of the rigid structure resisting the capillary forces during the evaporation. This was particularly evident in the 1:1 ration sample, which measured only 0.061 mm in thickness. While the 3:1 sample were somewhat more robust at 0.158 mm. As a result of this rigidity, both films performed poorly when subjected to bending forces, with the 3:1 film being somewhat more flexible than the 1:1 film, but still not comparable to the later ternary films.

3.2.2 Mechanical structure of MoS_2 films

The mechanical integrity of the binary MoS_2 films proved to be the most challenging aspect of their synthesis. While the 1:1 ratio film could be carefully handled, it was extremely brittle and would fracture immediately upon the application of any bending force. The 3:1 ratio film exhibited the worst structural integrity of all synthesised composites as they appeared fused to the bottom of the polystyrene petri dish. This indicated a strong interfacial bond between the almost empty CNC matrix and the substrate. Any attempts to extract the film resulted in it crumbling into small and unusable fragments, highlighting the lack of a cohesive internal network in the absence of the more stabilizing filler GO.

3.2.3 Homogeneous films and anchoring

The most significant finding of this thesis was the superior mechanical performance of the ternary 1:1 film. Unlike the binary MoS_2 films, the ternary composite did not adhere to the polystyrene substate, and unlike the GO films, it exhibited minimal coiling. Most notably, this specific film demonstrated the highest flexibility of all evaluated films, capable of being bent to an angle of approximately 90^{O} before snapping. This performance supports the hypothesis of a synergistic effect, where the GO sheets likely act as some type of anchor that stabilizes the MoS_2 flakes within the CNC matrix. This more entangled and cohesive network allows for a more effective distribution of mechanical stress, representing a stark improvement over the brittle behaviour observed in the binary equivalents.

3.3 Electrical properties

The electrical evaluation of the synthesised CNC composites revealed that all film variations, including the binary and ternary systems at both 1:1 and 3:1 ratio, remained in a strictly insulating state. In every instance, surface resistance measurements exceeded the maximum detectable limit of the multimeter, displayed as being 20 MΩ. Do note, this does not rule out semi-conductive properties that could exist beyond the 20 MΩ limit. Furthermore, this uniform lack of conductivity across all samples suggests that the functional additives did not reach the necessary percolation threshold required to form a continuous, electron-transporting pathway through the insulating CNC matrix.

The nonconductive behaviour of the CNC-GO components is specifically tied to the molecular hybridization of the graphene oxide. As established in the theoretical framework, the chemical oxidation procedure introduces a high density of oxygen-containing functional groups that convert the carbon atoms from a sp^2-hybridization state into a sp^3-hybridized configuration. This transition effectively breaks the "electronic highway" of graphene, trapping free electrons. Since the GO used in this thesis was not subjected to a subsequent reduction step to from reduced graphene oxide (rGO), it retained the insulation properties of its unreduced state.

While the ternary CNC-GO-MoS_2 films demonstrated superior macroscopic homogeneity and flexibility, the 1:1 and 3:1 additive concentration were not enough to overcome the combined effects of the broken π-conjugation in the GO and the semiconducting nature of MoS_2.

These results highlight that while the ternary system is a mechanical success, achieving electrical functionality would require either higher additive-to-CNC ratio or a chemical reduction process to restore the conductive sp^2-framework within the GO nanosheets.

4

Conclusion

The objective of this thesis was to investigate how Graphene Oxide (GO) and molybdenum disulfide (MoS_2) influence the films forming mechanisms and final physiochemical properties of a Crystalline Nanocellulose (CNC) matrix. By integrating theoretical principles of interfacial chemistry with our experimental findings, we have demonstrated that there are indications that the performance of these bio-based films is dictated by the specific molecular interactions between 1D and 2D nanomaterials.

4.1 The mechanical success of ternary synergy

The most significant finding of this research is the identification of a synergistic reinforcement effect within the ternary CNC-GO-MoS_2 system. While the binary composites suffered from either coiling (CNC-GO) or excessive substrate adhesion and brittleness (CNC-MoS_2), the 1:1 ternary hybrid exhibited superior structural integrity. Notably, this system achieved a bending threshold of approximately 90^{O} before snapping, a stark improvement over its binary counterparts.

This flexibility is attributed to the "anchoring" role of GO which utilizes its high-density hydrogen-bonding capacity to anchor MoS_2 flakes within the rigid CNC scaffold. This molecular interlocking creates a more entangled network that distributes mechanical stress more effectively the simpler binary composites.

4.2 The electrical challenge

Despite the mechanical gains, all synthesised films remain electrically insulating, with surface resistance exceeding 20 MΩ. This outcome in fundamentally tied to the chemical state of the additives and the concentrations thresholds within the matrix. The experimental data suggests that the functional additives did not reach the percolation threshold required to form a continuous conductive pathway.

Furthermore, the sp^3-hybridized domains within the unreduced GO effectively disrupts the delocalized π-conjugated system necessary for electron transport. Because the GO was not reduced to rGO to restore its sp^2-framework, it retained the insulating properties that define oxidized graphene.

While the ternary system is a success in terms of morphology and flexibility, its potential as an active electronic component remains dormant in its current unreduced state.

4.3 Future work

This thesis established a fundamental understanding of CNC-GO-MoS_2 ternary systems, but there still exists several possibilities for optimization and further investigation. They are as follows:

Improving statistical significance

To minimize the risk of outliers affecting the results and, in the process, enhancing the statistical significance, future studies should employ a larger sample size for each of the composite ratios. Moreover, investigating ratios where the filler is dominant instead of the CNC may yield interesting results regarding the loading limit before structural failure.

Quantitative characterization

As mentioned in section 1.2 *Limitations*, the qualitative assessments performed in this thesis should be explored with more standardized analytical instruments. Specifically, UV-VIS spectroscopy is recommended to give a quantifiable value to the optical transmittance, while analysis with dielectric spectroscopy would provide more objective data compared to the measurements with a multimeter.

Mechanical optimization

To combat the inherent brittleness of the formed CNC films, incorporating bio-based plasticizers could be explored. This would likely lead to improved flexibility and in turn make the films more suitable for different applications. Furthermore, an additional step where one reduces the films (chemically or thermally) could provide more conductive results via transitioning the GO to rGO.

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