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State of the Art and literature review research of Hollow Nanofibers: Focusing on fabrication, CAD implementation and optimisation

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Abstract. **The introduction of nanotechnology has resulted in a new era of materials research, with hollow nanofibers emerging as a key innovation. These nanofibers, distinguished by their nano size diameters and hollow structures, have generated significant interest due to their potential applications in a variety of industries. However, despite their advantageous properties, manufacture and analysis of these hollow nanofibers face significant challenges, particularly in terms of mechanical stability and structural integrity when subjected to external stresses. Identifying and addressing these vulnerabilities is crucial for the advancement of hollow nanofibers in various industrial and biomedical fields. The production of hollow nanofibers, notably via the electrospinning technique, has been the topic of a great deal of research. One of the bases of this research is the utilization of computer-aided analysis (CAD) simulations, which include techniques such as Representative Volume Element (RVE) analysis, Finite Element Method (FEM), multiscale analysis, numerical simulation, and optimization strategies. These sophisticated tools offer a magnified view into the nano-structural behaviour of hollow nanofibers, enabling precise predictions about their mechanical properties and behaviours under diverse conditions. This approach is revolutionary, as it allows for the exploration of theoretical and practical aspects of material behaviours without the constraints of traditional experimental methodologies. This article is in-depth scientific review on these theoretical and practical aspects.**

Keywords: Hollow nanofibers, Electrospinning process, Computer aided analyis.

I. INTRODUCTION

Nanofibers are fibers with diameters in the nano meter range, typically less than 100 nm. Due to their small size and high surface area-to-volume ratio, nanofibers are used in a variety of applications, including filtration, tissue engineering, and electronics. Hollow nanofibers, a subset of nanofibers, feature an empty core that enhances their functionality by reducing weight and increasing surface area, further broadening their applicative potential. Computer-aided analysis (CAD) of hollow nanofibers is crucial for optimizing their design and performance before physical prototypes are developed, saving time and resources in engineering processes. Writing a review on this topic is necessary to consolidate current knowledge, highlight advances, and identify gaps in the research, guiding future studies and technological development in this rapidly evolving field.

Firstly, this review briefly discusses about hollow nanofibers, electrospinning process strategies and the significance of CAD in hollow structures. Following that, this review focuses on the most recent advances in CAD for nanotechnology. At the end of this review, we explore and identify the challenges, opportunities, and future needs of CAD in hollow nanofibers.

II. METHODOLOGY: SCIENTIFIC LITERATURE REVIEW

A. Hollow nanofibers

The fabrication of hollow nanofibers has marked an important phase in materials research, motivated by nanotechnology's tremendous potential [1], [2]. These nanofibers, with their nanosized diameters and hollow centres ranging from 50 nm to 500 nm [3], [4], not only push the boundaries of material engineering, but also bring in a new era of innovation across a wide range of such as aerospace, automobile, military, sports, and biomedicine [5], [6]. Hollow nanofibers, with their unique structural properties such as high surface area-to-volume ratio, tenable porosity, and flexibility in functionalization, present a promising avenue for a plenty of applications in filtration methods [7]–[9], tissue engineering, drug delivery [10], [11], and more [12]–[14].

The potential of hollow nanofibers in catalysis, opens up new possibilities in chemical engineering and environmental science [15], [16]. These fibers enhance the efficiency of catalytic processes by providing a larger specific surface area, richer interfacial composition, and more efficient mass transfer paths, which are key to constructing multi-component catalytic systems and improving catalyst efficiency [17]. Hollow nanofibers have

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been found to substantially boost the efficiency of catalytic processes, with studies showing up to a 25% increase in catalytic efficiency compared to solid counterparts, primarily due to their expanded specific surface area that offers more active sites for reactions. Additionally, their unique interfacial composition enhances reactant interactions, while the hollow structure facilitates efficient mass transfer, potentially evidenced by a 40% increase in the turnover frequency (TOF) of catalysts, from 100 s^{-1} to 140 s^{-1} [18]. This illustrates how material innovations profoundly impact global challenges, as evidence materials science has played a key role in decreasing CO2 emissions from the electricity sector through the development of technologies for renewable energy generation and high-performance energy storage [19]. The exploration of core-shell nanofibers, with their complex design, expands the functional scope of hollow nanofibers by allowing the adjustment of their specific surface area and interface composition via their unique core-shell structure, resulting in an ideal platform for the preparation of highly efficient heterogeneous catalysts [20]–[23]. The layered design of these nanofibers significantly enhances their versatility, offering improvements in insulation, filtration, and protective coatings. For instance, the self-healing coatings containing core-shell nanofibers have demonstrated pH-responsive performance, with self-healing rates in acidic and alkaline solutions reaching 81.6% and 71.2%, respectively [24]–[27]. Additionally, making them particularly useful in advanced applications like gas sensing to detect SF6 decomposing gas products, thanks to their unique physicochemical properties [2], [23], [28].

In mechanical applications, the unique properties of polymer-based hollow nanofibers, such as their lightweight nature [6], offer significant advantages. For example, they have a larger surface area per unit mass and smaller diameter (10–100 nm), which contribute to their lightness. Their incorporation into composite materials can lead to innovations in lightweight construction such as the use of lightweight concrete, timber and bamboo composites, and fiber-reinforced polymers (FRPs) [29]. Structural integrity means that a structure or structural component is fit for purpose under normal operational conditions and is safe even should conditions exceed that of the original design [30]. This demonstrates their potential to improve performance in a variety of engineering applications and reduce energy consumption, as proved by an enhanced power conversion efficiency in polymer solar cells (PSCs) of up to 48.5% when compared to traditional bulk heterojunction solar cells [31].

Despite their promising characteristics, hollow nanofibers' mechanical stability under stress remains is a major concern [32]. One significant disadvantage is the potential for mechanical instability due to their thin-walled structure, which can lead to collapse under pressure or stress. From the studies, fibers having a diameter of 222-247 μm and a wall thickness of 50 μm can resist operating pressures of 20–25 bar for brackish water without collapsing [33]–[35]. The risk of structural collapse due to their thin walls limits their use in high-pressure conditions, up to 20-25 bar, emphasizing the need for additional research to improve their robustness by improving the wall thickness and overall dimensions [35]–[37]. The complexity of the manufacturing process for hollow nanofibers, which frequently results in such as irregularities in fiber diameter and wall thickness, with variations in the range of 5 to 15 μm for diameter and 180 to 900 nm for wall thickness [38], [39], [40]. These flaws are a significant barrier to achieving their full potential and can have a significant effect on hollow nanofiber performance in terms of mechanical stability, pressure resistance, and application efficiency [41]–[43]. This emphasizes the value of improving production procedures to assure the reliability and efficiency of hollow nanofibers in a variety of applications.

Fortunately, many previous review papers have discussed the fabrication of hollow nanofibers and their role in various applications, but from my literature survey, there are no review papers that systematically provide a review of the impact of CAD on hollow fiber structural design, optimization, prediction of mechanical behaviour, stability, and buckling. For instance, CAD simulations could lead to a 15% increase in mechanical strength and a 20% enhancement in stability against buckling, by optimizing fiber geometry and wall thickness. Hypothetically, nanofibers designed with CAD might show a tensile strength of 1.15 GPa compared to 1 GPa for traditionally designed fibers, highlighting CAD's role in improving nanofiber design and performance [44]. This gap in the literature presents an opportunity for in-depth research on CAD's contributions to nanofiber technology. To fulfil this gap my research empirically comparing the mechanical properties of CAD-designed nanofibers with those fabricated through traditional methods, researchers can substantiate the improvements and potentially establish new standards in nanofiber fabrication.

B. Fabrication

The hollow nanofibers are fabricated using electrospinning [45]–[48], a process that involves the use of two immiscible liquids through a coaxial, two-capillary spinneret, followed by selective removal of the cores. The methods used for the selective removal of the cores include wet, dry, melt, and gel spinning [13], [14], [49]. This technique has been demonstrated to be capable of producing hollow nanofibers with walls made of inorganic/polymer composites [12]. The size and wall thickness of these nanofibers can be independently varied by controlling a set of experimental parameters viscosity of the inner silicon oil phase [38], [50], [51]. The materials used for producing hollow fibers are typically polymer-based composites [52], [53] are chosen due to their unique properties such as lightweight, high stiffness, high specific strength, good resistance to fatigue, wear and corrosion resistance, easy fabrication, economic efficiency, high design flexibility, and desirable thermal expansion characteristics [54]. These properties make them suitable for various applications such as tissue engineering, wound dressings, drug release, regenerative medicine, dental resin composites and surgical operations [55]–[57].

In other studies, it was demonstrated that electrospinning involves carefully spinning two immiscible liquids (usually polymer solutions or melts and solvents such as limonene (CAS number: 138-86-3, MW: 136.23 g/mol), γ-valerolactone (CAS number: 108-29-2, MW: 100.12 g/mol), and 2-methyl tetrahydrofuran (2-MeTHF) (CAS number: 96-47-9, MW: 86.13 g/mol) [58] into fine nanofibers with a hollow core. It is crucial for the development of various innovative fibers, such as aligned, randomly oriented, core/shell, hollow, multichannel microtubes, colloidal nanoparticle-decorated, shish-kebab, helical, porous, necklace-like, island-like, and beads-in-fiber electrospun fibers [29], [59]–[61]. Adjustments in solution viscosity and electric field strength can produce nanofibers with diameters from 50 nm to 500 nm and increase surface area by up to 50%, enhancing their utility in applications such as filtration and drug delivery by providing a larger active surface for interactions [62]–[64]. This provides researchers an extensive tool for material design such as the synthesis of mesostructured nanofibrous mats for electrochemical energy storage devices, and the engineering of electrospun nanofibers as passive and active components for flexible/stretchable electronic devices [65]–[67]. It has gained attention for its ability to develop materials that could serve as the foundation for next-generation technologies [5], [68], [69]. Particularly in lightweight constructions such as tissue engineering, drug delivery, sensing, filtration, wound dressings, self-cleaning surfaces, biotechnology, environmental engineering, and green chemistry [60], [70], [71] and high-efficiency filters [72]–[74].

Precise manufacturing of polymer nanofibers, enables the manufacture of fibers specialized to specific needs, such as increased surface area for catalytic applications, which can be summarized as enhanced reactivity or controlled release in drug delivery systems including insulin, with precise control over the concentration and time of delivery [75], [76]. Depending on the specific use, the types of drugs, their concentrations, and delivery time can vary widely, but the main advantage is the maximization of therapeutic efficacy and minimization of off-target accumulation [2]. The basic characteristics of materials used to fabricate hollow nanofibers, particularly polymer-based composites, include synthetic polymers such as poly (lactic acid) (PLA), polycaprolactone (PCL), polyurethane (PU), poly (lactic-co-glycolic acid) (PLGA), poly (L-lactide) (PLLA), and poly (ethylene-co-vinylacetate) (PEVA) [77]. This advance their choice for a wide range of applications such as smart mats, catalytic supports, filtration membranes, energy storage/heritage components, electrical devices (batteries), and biomedical scaffolds [78]. These materials, known for their flexibility and adaptability, are crucial for achieving the desired functionality and performance of hollow nanofibers, such as high specific surface areas, superior mechanical properties, and outstanding flexibility of hollow nanofibers [17], demonstrating the crucial role of material selection in the success of these novel structures [77].

C. Role of CAD

The implementation of CAD simulations in the study of hollow nanofibers represents a paradigm shift in material research. This computational approach enables novel investigation of fiber nano and micro structures [79], resulting in a detailed understanding of their mechanical behaviour under various circumstances such as changes in temperature, pressure, and mechanical stress [77]. Such insights are invaluable in optimizing parameters like size, thickness and composition of the nanofiber characteristics for specific applications [2], bridging the theoretical-practical gap [78]. CAD simulations can predict the damage tolerance of these fibers in composite materials, guiding the development of products that are not only more resilient and durable [80]–[82]. Previous studies demonstrated that one specific model mentioned is for PANI (Polyaniline) hollow nanofibers. The model predicts that these nanofibers exhibit improved tensile strength by up to 40.3%, higher elasticity by up to 48.5%, and enhanced thermal stability [5].

The recent study on AlN/BN bishell hollow nanofibers, fabricated via electrospinning followed by atomic layer deposition, demonstrates a notable improvement in nanostructure composition and dimensions. The process achieved a uniform fiber diameter of approximately 100 nm and a significant structural integrity post-calcination at 500 °C, preserving the fibrous structure even after BN deposition. This advancement underscores CAD simulations' potential in enhancing the performance and scalability of nanofibers, providing a concrete example of how computational tools can guide material innovation in nanotechnology [80], [83], [84]. By establishing a virtual environment that emulates the electrospinning process [29], [85]–[87], researchers could identify and address potential flaws in fiber structure [88], [89], paving the way for the development of more durable and reliable nanofibers [32], [90]–[92]. Beyond design, CAD simulations are an effective tool for forecasting the mechanical properties of hollow nanofibers under various conditions including stress, strain, and environmental factors [93]–[98]. This feature is critical for adapting nanofibers to the precise needs of individual applications such as specific load-bearing requirements or flexibility parameters [99], ensuring their performance and stability in practical applications like filtration, energy storage, and biomedical devices [91].

CAD simulations are essential for determining the damage tolerance of hollow nanofibers in composite materials because they allow for the prediction and study of how these materials behave under stress, strain, and impact [100]. This ability to predict enables the development of materials that can resist tough conditions such as high pressures, extreme temperatures, and corrosive environments [101], [102], these vital factors in industries such as aerospace and automotive, where material failure can have significant implications [103]. These industries require materials that not only perform reliably but also ensure safety and longevity of the components made from them. CAD's contribution to enhancing the mechanical characteristics of hollow nanofibers is invaluable the ability to model and simulate various structural and material properties, such as tensile strength, elasticity, and thermal stability. This enables the optimization of nanofibers for specific applications by adjusting parameters like fiber diameter, wall thickness, and composition to achieve the desired performance [5]. By offering precise control over fiber design and qualities [104]–[106], CAD offers that nanofibers may meet the demanding standards of complicated uses ranging from high-strength materials like advanced composites and alloys. Carbon fiber-reinforced polymers and titanium alloys, crucial in aircraft and high-performance vehicle construction [107], to flexible electronic devices such as wearable sensors, flexible displays, and bendable batteries, which demand materials capable of maintaining functionality under bending or twisting [108]–[110].

III. Discussions

A. Approach: CAD-Driven Optimization of Hollow Nanofibers for Aerospace Applications

The potential use of hollow nanofibers in aircraft composites is very fascinating because these materials offer a unique combination of lightness and strength, which are paramount in aerospace engineering [111], [112]. Here, CAD simulations help build materials that balance weight and strength [113], which is crucial in aerospace engineering where every gram counts, illustrating the innovative influence of material finds in high-stakes industries. From my literature survey, the integration of CAD simulations has been transformative in this field, enhancing the precision in design and optimization of these nanomaterials. CAD's contribution has been particularly notable in refining the nanostructure composition and dimensions of hollow nanofibers, crucial factors for their performance and scalability. Specifically, CAD simulations have facilitated a 30–40% enhancement in the tensile strength and elasticity of nanofibers. This improvement stems from this approach of optimized nanostructure design that minimizes the risk of mechanical failure under stress, thereby boosting the fibers overall durability and performance. Additionally, CAD's influence on material selection and structural design has improved the manufacturability and scalability of hollow nanofibers by 20–25%, making them more suitable for widespread industrial use [114]. Hollow nanofiber research is essentially interdisciplinary, integrating insights from material science, chemical engineering, and computational modelling [115]–[118]. This collaborative approach is critical in pushing the limits of what is feasible with these materials [119], [120], potentially leading to breakthroughs that change the landscape of modern technology, particularly in fields where material efficiency and performance are crucial [121], [122]. For instance, in the aerospace industry, innovations could result in lighter, more fuel-efficient aircraft. Hollow nanofibers could help to produce lighter, more efficient, and perhaps more powerful batteries and supercapacitors, with implications for anything from consumer electronics to electric vehicles [123].

B. Gaps and Challenges

From my research, hollow structured nanofibers present unique advantages but are accompanied by significant challenges, such as reduced mechanical strength due to thin walls, susceptibility to buckling, complex geometry in design, and assembly difficulties. CAD simulations offer solutions to these challenges by enabling predictive modelling to optimize mechanical behaviour, stability, and wall thickness. They facilitate precise structural design, taking into account material distribution and load requirements, and assist in visualizing assembly processes to pre-empt potential issues. Furthermore, CAD tools support the selection of appropriate materials, enhancing the safety, performance, and manufacturability of hollow nanofibers. Through the strategic use of CAD, engineers can effectively navigate the complexities associated with hollow nanofibers, ensuring their practical application across various fields.

C. Future Scope

A Future research areas include optimizing the electrospinning method for hollow nanofibers, with a focus on attaining more control over fiber properties such as their high specific surface areas, high surface area to volume ratios, easy functionalization, superior mechanical properties, outstanding flexibility, controllability in fiber diameter, surface morphology, and fibrous structure [124]–[126]. CAD simulations offer a pathway to study and resolve these unsolved issues such as humidity in the electrospinning environment, beading of fibers spun at two different viscosity solutions, poorly aligned fibers, uneven diameters, slow drum RPM, unstable drum, airflow in the electrospinning environment disrupting the jet, and fluctuating temperature in the electrospinning environment [127], [128]. By simulating the electrospinning process and the resultant fiber morphology, researchers can identify and mitigate potential points of failure in the fiber structure [129]–[131]. This endeavour will most likely include experimenting with novel materials and process parameters in order to reduce flaws and enhance fiber functionality [132], [133]. The search for materials with superior properties like mechanical strength [134], [135], chemical resistance [136], [137], or biocompatibility [138]–[140], will drive advances in nanofiber applications ranging from biomedicine to sustainability a career in engineering [141], [142].

CAD tools are essential for advancing hollow nanofiber research due to their ability to model and simulate complex material behaviours and processing conditions such as temperature variations, humidity levels, and the dynamics of electrospinning, with precision with precision. These tools will need to simulate increasingly complex phenomena within nanofibers [106], accommodating the growing sophistication of research questions such as the impact of environmental factors on nanofiber morphology [77], the role of solution viscosity in fiber formation[138], and the influence of process parameters on fiber alignment [143]. The need for more nuanced analyses could include the study of the effects of humidity [5] and temperature on the electrospinning process, the investigation of the mechanical behaviour of nanofibers under various conditions, and the prediction of damage tolerance of nanofibers in composite materials [144], [145].

IV. Conclusion

In conclusion from the summary of literature overview, hollow nanofibers hold great promise for material innovation, but realizing their full potential hinges on a comprehensive understanding and improvement of their properties such as mechanical strength, thermal stability, and electrical conductivity. The collaborative effort of material scientists, engineers, and computer modelers, supported by the vital role of CAD simulations, is critical to the advancement of hollow nanofiber technology. This interdisciplinary collaboration, along with the precision delivered by CAD in designing and refining the geometry of fibers, is driving novel solutions, new applications, and enhanced understanding of these materials. CAD's role in accurately modelling the 2D and 3D aspects of fiber structure enables engineers to develop more effective and innovative uses for hollow nanofibers. In industries such as aerospace, where the balance of material efficiency and strength is critical, CAD's ability to optimize the mechanical properties of nanofiber-reinforced composites is proving crucial demonstrating the important role of these collaborations in pushing the boundaries of material science. Future research should concentrate on fortifying the mechanical stability of these fibers and extending their use in mechanical applications through the application of sophisticated CAD techniques. The literature review underscores the importance of CAD simulations in advancing the field of hollow nanofibers and highlights the need for continued research to overcome the current limitations and unlock new possibilities for their use.

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