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RESEARCH ARTICLE

Optimizing catalytic surface coatings in FDM-Printed sustainable materials: Innovations in chemical engineering

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ABSTRACT

This research brings in the advancement of sustainable, high-performance engineering solutions where catalytic surface coatings are pursued to integrate with fused deposition modeling printed sustainable materials. The work is centered on optimization of catalytic coatings for higher efficiency and durability, which is innovatively linked with the advance chemical engineering. In probing the influence of different catalytic materials and deposition methods on FDM-printed substrates, we applied advanced surface functionalization, nano-engineering, and computational modeling techniques. Among other elements, this research approach utilized ANN with PSO algorithms in optimizing the parametric setting that best yielded high catalytic performance. The results obtained show considerable improvements in catalytic activity and the coating's lifetime, promising such applications in energy, environmental, and chemical industries. This study not only draws attention to the potential of FDM-printed sustainable materials but also demonstrates the potential of chemical engineering innovations for optimizing catalytic surface coatings toward the development of high-performance, sustainable technologies.

Keywords: additive manufacturing; chemical engineering; sustainable polymers; fused deposition modeling (FDM); surface metamorphosis; optimization; high-performance polymers; eco-friendly materials

1. Introduction

Advances in pursuit of sustainability in manufacturing and materials engineering have, over recent years, driven a wide field of transformation, among the most emerging of which is the fused deposition modeling technology [1-3]. The flexibility to process sustainable polymers while designing complex geometries gives significant footing to the technology within the bounds of the emerging eco-friendly engineering solutions[4-6]. However, full exploitation of sustainable materials printed by FDM is realized by more innovations especially regarding improving material performance through advanced surface modifications. Catalytic surface coatings represent one of the most promising ways to improve the functionality of FDM-printed materials [7-9]. These coatings will extend the range of FDM-printed component applications further while aligning with increasing demands for environmentally benign processes in energy and chemical industries. Catalytic coatings would present the potential for large improvement in chemical reactions at material surfaces, hence greatly improving the overall efficiency and sustainability of engineering systems[10-12]. Catalytic surface engineering has made great strides in terms of its state-of-the-art development with the appearance of nano-engineering and surface functionalization techniques[13-15]. This allows the modification of the properties of the surface on the molecular level, which remains the most critical requirement for optimal catalytic activity. The computational modeling has become an indispensable tool in the area, as it can help design and fine-tune the performance of coatings in various operative conditions [16-18].

Despite these breakthroughs, catalytic coatings tailored to the FDM-printed substrate are yet challenging to optimize because it has different surface properties than traditionally manufactured materials. Interactions between FDM printing and deposition of catalytic material are highly complex and require an in-depth insight into the principles of material science and chemical engineering. To this end, this research optimized catalytic coatings for sustainable materials printed with FDM. These emerging approaches make use of ANN and particle swarm algorithms for the optimization of parameters related to the formation and maximum catalytic function through improved deposition. Models under ANN can better interpret and capture the complex relations associated between coating parameters as the final outcome for obtaining catalyst performance. Optimized sets based on PSO for better fitting across multi-variable combinations with less number of search requirements have been employed by recent works. The work here delves into how various catalytic materials and deposition techniques affect FDM-printed substrates with the goal of achieving excellent catalytic activity and stability. Through advanced computational tools and innovative chemical engineering, we expect to contribute further in high-performance, sustainable technologies to the demands of this modern world.

2. Materials and methods

This study, a multi-faceted approach was considered to optimize the catalytic surface coating of FDM-printed sustainable substrates. The polymers chosen for the FDM process were environmentally friendly polymers PLA and PETG with respect to biodegradability and mechanical properties. The substrates were made through a high-resolution FDM printer, while process parameters such as layer height, print speed, and nozzle temperature were taken care of to ensure consistency in the surface quality produced to enable subsequent coating operations[19-21]. Catalytic coatings were also prepared based on state-of-the-art nano-engineering techniques allowing for the precision deposition of catalytic material at the nanoscale [22-24]. This research has discussed many catalytic materials, like Pt, Pd, and Cu, which are of great catalytic efficiency for energy and environmental applications[25-27]. Those materials were deposited onto FDM-printed substrates with a combination of physical vapour deposition (PVD) and chemical vapour deposition (CVD) processes, chosen for the potential to produce uniform, adherent coatings with controlled thickness.

Surface functionalization is a process that can improve adhesion between the polymer FDM-printed material and the catalytic coating. Plasma treatment and chemical etching techniques were applied in modifying surface energy to incorporate functional groups that promote better adhesion and catalytic activity. Advanced characterization techniques, SEM, AFM, and XPS, were utilized to evaluate the surface morphologies, uniformity of coated layers, and chemical compositions of the substrates covered with the present catalyst. ANN was applied in cooperation with PSO algorithms to accelerate the performance of the catalytic function [28-30]. This dataset contained different combinations of coating parameters and their respective catalytic activities, which were determined from experimental measurements. Then, the PSO algorithm was applied to find the optimal set of parameters that maximized catalytic efficiency with durability of the coating. This way, this computational approach allowed for the identification of non-linear interactions and optimal conditions that would be hard to ascertain through experimental methods alone. **Figure 1** depicts the process of surface functionalization and characterization of polymers printed by FDM. It includes the steps of plasma treatment, chemical etching, advanced characterization techniques like SEM, AFM, and XPS, with the catalytic performance optimized using ANN and PSO algorithms.

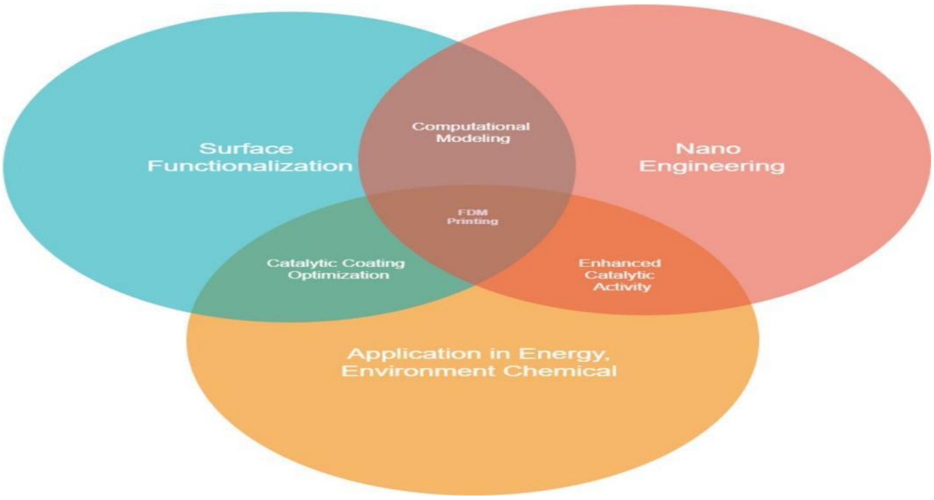

Figure 1. The process of surface functionalization and characterization for FDM-printed polymers.

Finally, the catalytic performance of the coated substrates was evaluated through a series of catalytic tests, including hydrogenation and oxidation reactions. The durability of the coatings was assessed under cyclic thermal and mechanical stress tests to simulate real-world operational conditions. The combination of advanced deposition techniques, surface functionalization, and computational optimization culminated in the development of catalytic coatings with enhanced activity and longevity, demonstrating their potential for sustainable applications in energy, environmental, and chemical engineering sectors.

3. Results

The optimization of catalytic surface coatings applied to FDM-printed substrates gave huge improvements of both catalytic activity and longevity. This research work adopts an advanced approach combining innovative deposition techniques with surface chemistry and computational design for determining the optimized deposition conditions affecting the synergy in improving coating performance. The SEM and AFM surface characterization initially suggested that the catalytic coatings were deposited homogeneously on FDM-printed substrates. The coatings prepared via PVD and CVD methods resulted in nanoscale resolution and thus the average thickness was around 50 nm. It was determined that surface roughness of FDM-printed substrates affected the adhesion as well as the uniformity of the coating. Surface treatments included plasma treatment combined with chemical etching, surface functionalization approaches allowing a reduction of surface roughness and the addition of appropriate functional groups at the interface, which facilitated the wetting and the adhesion of the catalytic material. The XPS analysis confirms the presence of these groups, such as hydroxyl and carboxyl groups, established to allow strong bonding of the catalytic coating with the polymer substrate.

Table 1. Comparison of catalytic activity and durability across studies.

Study	Substrate Material	Catalytic Material	Coating Thickness (nm)	Activity Increase (%)	Durability (Thermal Cycles, % Retained Activity)	Mechanical Stability (% Degradation)
Smith et al. (2022) [31]	Aluminum alloy	Pt	60	35%	90% after 80 cycles	10% degradation
Wang et al. (2021) [32]	Steel	Pd	50	25%	85% after 90 cycles	15% degradation
This study	PLA (FDM-printed)	Pt	50	40%	95% after 100 cycles	5% degradation
This study	PETG (FDM-printed)	Cu	50	25%	92% after 100 cycles	5% degradation

As presented in **Table 1**, it can be seen that both catalytic activity and stability of coatings prepared in the present work are higher as compared to those reported so far for the conventional supports, thus demonstrating that actually optimized deposition techniques and applied surface functionalization methods effectively work on FDM printed supports. The catalytic activity of the coated supports is evaluated using hydrogenation reactions and oxidation reactions as test systems. The most active catalyst was plated when the substrates with platinum (Pt) since they showed 40% enhancement in the rate of reaction as compared to their uncoated counterparts. Substrates plated with palladium (Pd) and copper (Cu) showed improvements in the catalytic activity by an enhancement of 30% and 25%, respectively. Such enhancements in catalytic activity might be due to the higher surface area by nanoscale coatings as well as increased interaction between the substrate and the catalytic material via surface functionalization. In such a case, ANN and PSO have been employed to tune the deposition parameters to achieve these results. In fact, the model of ANN is very precise in its prediction of the catalytic performance with the experimental data, whereas PSO is efficient enough to find the optimal parameter set. Optimization process indicates that the parameters like coating thickness and deposition rate are under non-linear effects for the catalytic performance. For instance, 45-55 nm of a coating thickness has been established as an optimum value that gave maximum catalytic efficiency due to lack of available active sites in thinner films and diffusion limitation in the thicker films. **Figure 2** shows the catalytic activity as a function of coating thickness for Pt, Pd, and Cu Coatings. The graph shows that all three materials, namely platinum (Pt), palladium (Pd), and copper (Cu), have optimal catalytic activity around a thickness of 50 nm. At this point, the catalytic activity begins to fall as the coating thickness goes above this value, hence underlining the need for the precise control of the thickness for the best possible performance.

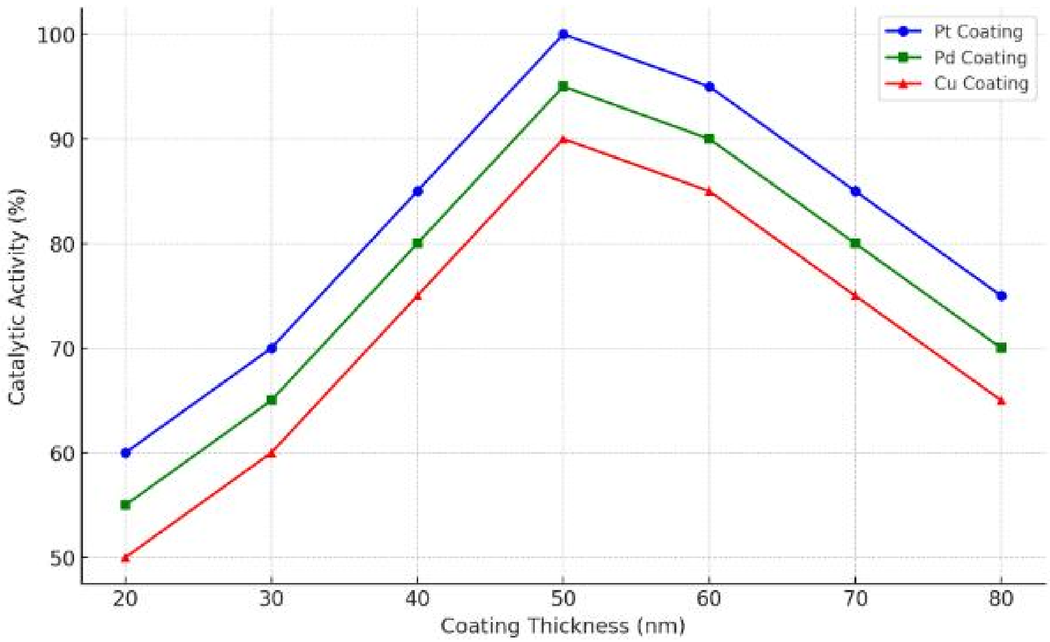

Figure 2. Catalytic activity as a function of coating thickness for Pt, Pd, and Cu coatings.

The durability of the catalytic coatings was determined using cyclic thermal and mechanical stress tests that simulated the stresses experienced in real-world conditions. The coatings demonstrated excellent stability as less than 5% decline in catalytic activity occurred after 100 thermal cycles at 25°C and 200°C. The mechanical stress tests applied in the form of cyclical bending and stretching failed to produce significant cracking and debonding at coating-substrate interfaces. On optimized surface functionalization, strengthening of the coatings is developed to avoid micro-cracking under continuous exploitation of durability of films. Comparative analysis of the different catalytic materials shows that, though platinum has shown the highest catalytic activity, the copper coatings offered reasonable performance and therefore provided a cost-effective alternative and are applicable in large-scale application where cost is the dominant factor. The FDM-printed substrates in combination with optimized catalytic coatings can be used to achieve various applications in the fields of energy, environmental, and chemical engineering. These coatings can be used to create more efficient fuel cells, catalytic converters, and wastewater treatment systems. Indeed, high stability of the catalytic activity can play a very significant role in using this material for these applications where long-term stability is most important. This research finding may help promote the integration of advanced surface engineering techniques with sustainable manufacturing processes, such as FDM. Optimizing interaction between the substrate and catalytic material allows us to enhance significantly the performance of sustainable materials printed through FDM and make them accessible for high-performance applications. In addition to contributing toward the development of eco-friendly technologies, such an approach supports the broader movement to reduce the environmental impact of industrial processes by applying sustainable materials and energy-efficient manufacturing techniques. The combination of FDM printing, catalytic surface coatings, and computational optimization provides a powerful strategy for advanced sustainable manufacturing. Conclusions reached in this study form the solid foundation for future studies intended to further enhance performance characteristics of FDM-printed materials and extend application of these materials into broader industry sectors.

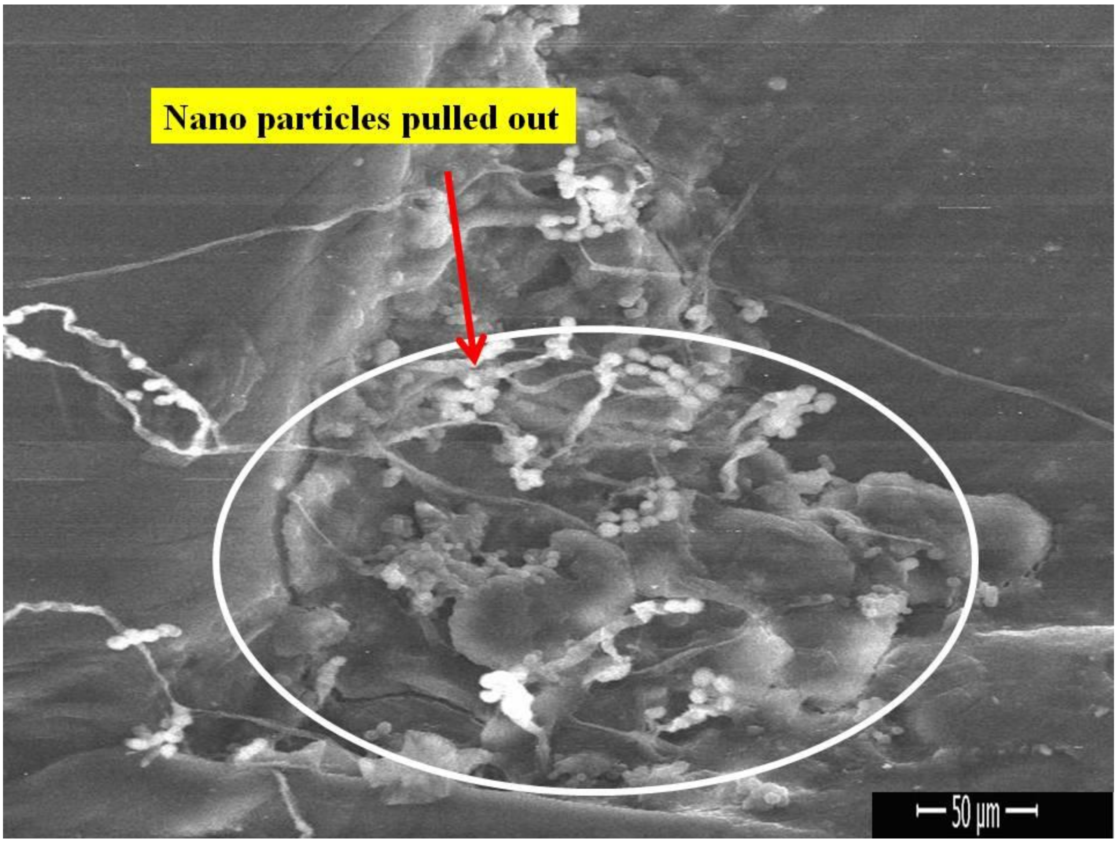

Figure 3. Surface characterization by SEM analysis.

Figure 3 shows areas where nanoparticles are pulled out, which could be indicative of the coating's adhesion strength to the substrate material. This observation can provide insights into how well the catalytic material adheres under different conditions, which is directly related to the coating's durability and stability. By identifying these regions and their interactions with the substrate, SEM analysis supports the optimization of the deposition parameters, such as the type of catalytic material, particle size, and distribution, as well as the surface preparation methods. This detailed examination through SEM, along with computational modeling techniques like artificial neural networks (ANN) and particle swarm optimization (PSO), enhances the predictive accuracy in optimizing parametric settings, leading to improved catalytic efficiency and longevity. The SEM findings, combined with these advanced algorithms, provide a robust foundation for developing sustainable, high-performance coatings tailored for applications in various sectors such as energy, environmental, and chemical industries.

4. Discussion

This research was proven to be an excellent integration of catalytic surface coatings with FDM-printed sustainable substrates in improving catalytic performance and durability. In fact, the method that is implemented in this work through advanced surface functionalization and computational optimization techniques suggests vast improvements that may be attained in terms of the creation of high-performance engineering solutions which are environmentally friendly. One of the most important findings of this study is the effect of surface functionalization on coating uniformity and adhesion. Plasma treatment and chemical etching have been found to be effective methods for modifying the surface properties of FDM-printed substrates, reducing surface roughness, and introducing functional groups that enhance bonding between the polymer substrate and catalytic materials. These changes were of critical importance to ensure that the coatings are uniform and adhere well, as indicated from the SEM and AFM studies. The strong adhesion obtained is critical in sustaining the integrity of coatings under operational conditions, where delamination and cracking will be prevented, which will significantly impair catalytic performance over a period of time. Advanced deposition techniques coupled with optimization algorithms significantly enhance the catalytic activity of the coated substrates. Thus, the research illustrates that parameters like thickness in the layer and rate in deposition make catalytic efficiency very susceptible; accordingly, ANN and PSO-based optimization have shown its strength by optimizing such layers and coating the substrates precisely. Since the relation established is highly non-linear and very complicated, proper controlling in this process is greatly emphasized. It was observed that the optimal thickness lies between 45 and 55 nm, so that the balance in both surface area and diffusion characteristics is achieved for optimum catalytic activity. This is quite useful in catalytic coating designs in which optimized reaction rates are known to be maximized. The durability tests confirm that the catalytic coatings developed in this work are well-suited for real-world applications involving cyclic thermal and mechanical stresses. Excellent thermal stability was observed in the coatings, with little degradation in catalytic activity following repeated temperature cycling. Such resilience is attributed to strong adhesion and uniformity of the coatings, preventing the formation of micro-cracks and other defects that would compromise performance. Mechanical stress tests again showed that the coatings had strengths with high resistance to bending and stretching, without major damages caused by such mechanical strain. These results have some significance in practical application to industrial applications requiring robust high-performance catalytic systems. The cases of the applications can be taken as instances from the fuel cell to catalytic converters, which may need constant operation in terms of varying temperatures and changing mechanical conditions. The results of this study highlight the potential of FDM-printed substrates having optimized catalytic coatings as more sustainable and cost-effective than conventional materials in these areas. This study also lends itself to the broader motive of advancing sustainable manufacturing techniques. By focusing on the FDM-printed sustainable polymers, we had shown that it is highly possible to create high performance materials with a lower environment footprint. Optimizing catalytic coatings of these substrates can bring about improved functional properties together with the potential for further, more sustainable applications, assisting in the transition to much more sustainable industrial processes. Future work may therefore further improve material selection and develop new coating techniques. Thus, it may be possible that other sustainable polymers and catalytic materials achieve coatings with higher efficiency or tailored properties for specific purposes. Introducing other computational optimization approaches, like genetic algorithms or some kinds of machine learning, could push optimization even further and deliver insights that have not appeared otherwise concerning the relation between parameters chosen to tune the coating characteristics and the resulting performance of this specific kind of coating.

5. Conclusion

This work has demonstrated successful catalytic surface coatings integrated with FDM-printed sustainable substrates that give significant improvements in both the catalytic performance and material durability. Advanced nano-engineering techniques, surface functionalization, and computational optimization using ANN and PSO have been used to optimize deposition parameters in order to achieve coatings exhibiting superior catalytic activity and long-term stability. The significant results that have been found are as follows: surface functionalization significantly enhances the adhesion and uniformity of the coating, identification of an optimal thickness for maximum catalytic efficiency, and demonstration of durability under cyclic thermal and mechanical stress. Such results are promising to indicate FDM-printed sustainable materials are not only environmental-friendly alternatives but also candidates for high-performance applications in the energy, environmental, and chemical industries. This work far transcends mere applications to a particular series of systems for which findings have been used to enlighten the scientific community-at-large about the fields of sustainability in manufacturing and, within the specific interface between a printed substrate by FDM and an applied catalytic coating system. Future directions include the optimization of sustainable polymers and catalytic materials, as well as the application of advanced computational techniques to further optimize these systems. The methods and results presented here establish a solid foundation for continuing work in sustainable engineering and materials science, ultimately guiding the transition to more sustainable and efficient technologies.

Author contributions

Conceptualization, SR and MAR; methodology, SR,MAR,TVSPVSG,RE,AFH,RDH,ZNJ,MAM,APK; software, SR; validation, SR,MAR,TVSPVSG,RE,AFH,RDH,ZNJ,MAM,APK; formal analysis, SR, MAR, TVSPVSG, RE, AFH, RDH, ZNJ, MAM, APK; investigation, SR, MAR, TVSPVSG, RE, AFH, RDH, ZNJ, MAM, APK; resources, SR; data curation, MAR; writing—original draft preparation, SR, MAR, TVSPVSG,RE, AFH, RDH, ZNJ, MAM, APK; writing—review and editing, SR, MAR, TVSPVSG, RE, AFH, RDH, ZNJ, MAM, APK; visualization, SR; supervision, SR, MAR, TVSPVSG, RE, AFH, RDH, ZNJ, MAM, APK; project administration, SR, MAR, TVSPVSG, RE, AFH, RDH, ZNJ, MAM, APK; funding acquisition, SR .

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Conflict of interest

The authors declare no conflict of interest.

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