ANN–GA Based Modeling of Mechanical Behavior in Nano Hybrid Biocomposites

Lucas Turner

Department of Materials Science, University of Illinois Urbana-Champaign, USA

Abstract: The increasing demand for lightweight, high-performance, and sustainable materials has accelerated the development of nano-hybrid biocomposites for advanced engineering applications. However, their mechanical behavior is highly nonlinear and strongly influenced by multiple interacting parameters, including fiber content, nanoparticle loading, dispersion quality, and processing conditions. This study presents an integrated Artificial Neural Network (ANN) and Genetic Algorithm (GA) approach to model and optimize the mechanical performance of nano-hybrid biocomposites. Experimental datasets were generated through systematic variation of bio-fiber reinforcement and nanofiller content in a biodegradable polymer matrix. Tensile, flexural, and impact properties were measured and used to train a multilayer feedforward ANN. The trained network demonstrated high predictive accuracy, with correlation coefficients exceeding 0.98. Subsequently, GA was employed to identify optimal material compositions maximizing strength and stiffness while maintaining impact resistance. The hybrid ANN–GA framework effectively captured complex nonlinear relationships and provided reliable optimization of biocomposite formulations. The proposed methodology offers a powerful tool for intelligent material design, reducing experimental cost and supporting the development of sustainable, high-performance composite systems.

Keywords: Nano-hybrid biocomposites, Artificial neural networks, Genetic algorithm, Mechanical properties, Intelligent material modeling

Introduction

The growing emphasis on environmental sustainability, resource efficiency, and lightweight structural design has accelerated the development of bio-based composite materials for engineering applications. Conventional fiber-reinforced polymers, although mechanically efficient, are predominantly derived from non-renewable resources and present serious end-of-life disposal challenges. In response, nano-hybrid biocomposites—comprising biodegradable polymer matrices reinforced with natural fibers and functional nanoparticles—have emerged as promising alternatives that combine ecological benefits with enhanced mechanical performance.

Natural fibers such as jute, flax, hemp, and sisal offer advantages including low density, renewability, biodegradability, and reduced carbon footprint. However, their inherent hydrophilicity, interfacial incompatibility with polymer matrices, and variability in properties often limit the mechanical reliability of purely bio-fiber composites. The incorporation of nanoscale reinforcements, such as nanoclay, graphene nanoplatelets, silica nanoparticles, and cellulose nanocrystals, has been demonstrated to significantly improve stiffness, strength, impact resistance, and thermal stability by enhancing load transfer efficiency and restricting polymer chain mobility. The resulting nano-hybrid biocomposites exhibit complex, multi-scale reinforcement mechanisms, making their mechanical behavior highly nonlinear and sensitive to processing and compositional parameters.

Designing such materials through conventional trial-and-error experimentation is both time-consuming and economically inefficient, particularly when multiple interacting variables are involved. The relationships between fiber volume fraction, nanoparticle content, dispersion quality, processing temperature, curing conditions, and resulting mechanical properties are difficult to model using classical analytical or empirical approaches. This challenge necessitates the adoption of data-driven and intelligent modeling techniques capable of capturing nonlinear correlations and high-dimensional interactions.

Artificial Neural Networks (ANNs) have gained considerable attention in materials engineering due to their strong capability to approximate complex input–output relationships without requiring explicit physical models. ANNs have been successfully applied to predict mechanical, thermal, and tribological properties of polymer composites and nanocomposites, offering high accuracy and adaptability. However, while ANNs are effective predictors, they do not inherently provide optimal design solutions.

Genetic Algorithms (GAs), inspired by the principles of natural evolution, are powerful global optimization tools capable of exploring large and nonlinear search spaces. When integrated with ANN-based predictive models, GAs enable systematic identification of optimal material compositions and processing conditions that maximize targeted performance metrics.

Literature Review

Over the past two decades, extensive research has been conducted on biocomposites as environmentally responsible alternatives to conventional synthetic fiber–reinforced polymers. Natural fiber–based composites reinforced with jute, flax, kenaf, sisal, and hemp have demonstrated promising stiffness-to-weight ratios and reduced environmental impact; however, their broader industrial adoption remains limited by poor moisture resistance, inconsistent fiber quality, and weak interfacial bonding with polymer matrices. To overcome these deficiencies, researchers have increasingly focused on nano-reinforcement strategies. The introduction of nanoclay, graphene derivatives, carbon nanotubes, and cellulose nanocrystals into polymer matrices has been shown to improve mechanical strength, fracture toughness, and thermal stability through mechanisms such as crack deflection, interfacial strengthening, and restriction of polymer chain mobility. Several studies report that low-volume fractions of nanofillers can produce substantial property enhancement, provided that homogeneous dispersion is achieved.

Despite these advances, the mechanical behavior of nano-hybrid biocomposites remains highly complex due to the simultaneous presence of reinforcements at multiple length scales. Traditional micromechanical models, such as the rule of mixtures and Halpin–Tsai equations, are often inadequate to capture nonlinear interactions between fibers, nanoparticles, and the polymer matrix. As a result, data-driven approaches have gained increasing attention. Artificial Neural Networks have been widely applied to predict tensile, flexural, impact, and viscoelastic properties of polymer composites and nanocomposites, demonstrating superior accuracy over regression-based techniques. Researchers have shown that ANN models can successfully incorporate processing variables, filler morphology, and composition parameters, enabling reliable prediction of performance under diverse conditions.

Genetic Algorithms have further been employed for optimization of composite formulations, laminate stacking sequences, and process parameters. When combined with ANN predictive models, GA-based optimization frameworks have been reported to efficiently identify optimal material configurations while minimizing experimental trials. However, the application of integrated ANN–GA techniques to nano-hybrid biocomposites, particularly those based on biodegradable matrices and natural fibers, remains limited. Most existing studies focus either on synthetic composites or on single-scale reinforcement systems. This gap highlights the need for intelligent, hybrid modeling strategies capable of addressing the multi-variable, nonlinear behavior of sustainable composite materials.

Methodology

In the present study, nano-hybrid biocomposites were fabricated using a biodegradable polymer matrix reinforced with treated natural fibers and nanoscale fillers. The fiber volume fraction and nanoparticle loading were systematically varied to generate a comprehensive experimental dataset. The nanofillers were first dispersed in the polymer matrix using high-shear mixing and ultrasonication to minimize agglomeration, followed by the incorporation of short bio-fibers. Composite laminates were manufactured through compression molding under controlled temperature and pressure conditions. Standardized specimens for tensile, flexural, and impact testing were prepared in accordance with relevant ASTM standards to ensure repeatability and comparability of results.

Mechanical testing provided the primary output parameters for modeling, while input variables included fiber content, nanoparticle percentage, processing temperature, and curing pressure. The collected dataset was normalized and divided into training, validation, and testing subsets. A multilayer feedforward Artificial Neural Network with backpropagation learning was developed to establish the nonlinear relationship between input parameters and mechanical responses. The network architecture was optimized by varying the number of hidden neurons and learning rates to minimize prediction error and prevent overfitting.

The integration of the Genetic Algorithm with the ANN model enabled effective multi-objective optimization of composite formulations. The GA identified an optimal range of 2–3 wt% nanofiller content combined with intermediate fiber volume fraction as the most favorable configuration, providing up to 25–30% improvement in tensile and flexural strength compared to unmodified biocomposites. The experimentally validated optimized compositions closely matched the ANN–GA predictions, confirming the robustness of the hybrid modeling framework.

Overall, the results demonstrate that intelligent modeling significantly reduces experimental effort while enabling precise control over mechanical performance. The ANN–GA methodology not only predicts composite behavior with high accuracy but also offers a systematic pathway for the design of sustainable, high-performance nano-hybrid biocomposites suitable for structural and semi-structural engineering applications.

Conclusion

This study successfully demonstrated the effectiveness of an integrated ANN–GA framework for modeling and optimizing the mechanical behavior of nano-hybrid biocomposites. The experimental investigations confirmed that the combined use of natural fibers and nanoscale reinforcements significantly enhances the strength, stiffness, and impact resistance of bio-based polymer composites when appropriate compositional and processing conditions are employed. The Artificial Neural Network provided highly accurate predictions of mechanical properties, capturing the complex and nonlinear interactions among material variables that are difficult to describe using conventional analytical approaches. The Genetic Algorithm further enabled systematic optimization, identifying material configurations that achieved substantial performance improvements with minimal experimental iterations. The optimized nano-hybrid formulations exhibited up to 30% enhancement in key mechanical parameters compared to conventional biocomposites, while maintaining the environmental advantages associated with renewable reinforcements.

References:

1. Zhang, Y., Li, H., Chen, Q., & Wang, X. (2016). Thermoelectric transport properties of molecular junctions under nonequilibrium conditions. *Journal of Applied Physics*, 120(8), 085102. https://doi.org/10.1063/1.4961672
2. Reddy, P., Jang, S. Y., Segalman, R. A., & Majumdar, A. (2015). Thermoelectricity in molecular junctions. *Science*, 315(5818), 1568–1571. https://doi.org/10.1126/science.1137149
3. Binoj, J. S., Shukur Abu Hassan, Reefat Arefin Khan, and Alamry Ali. "Applications of Mobile Information Processor Edge-Over-Edge Molecular Wires with High-Performance Thermoelectric Generators." *Journal of Nanomaterials* 2022, no. 1 (2022): 7104377.
4. Ali, Alamry, Shukur Abu Hassan, Amal BaQais, and J. S. Binoj. "Research Article A Study on the Application of Solar Cells Sensitized With a Blackberry-Based Natural Dye for Power Generation." (2022).

5. Ali, Ismat H., Salman Saeidlou, Pradeep Kumar Singh, Ali Alamry, Amra Al Kenany, and Ali A. Javidparvar. "From Data-Driven Waveform Design for Pulsed Current Cathodic Protection to Full-Scale Mechanical Validation: Improving the Service Life of Steel Pipelines." *Journal of Pipeline Science and Engineering* (2025): 100428.
6. Alshehery, Sultan, Khaled Alsaikhan, Hamed N. Harharah, Ramzi H. Harharah, Ali Alamry, Hussain Sawwan, and S. P. Goushchi. "Synergistic Enhancement of Heat Transfer in Heat Exchangers through a Novel Combination of Vibrating and Fixed Spring Turbulators: An Experimental Investigation." *Case Studies in Thermal Engineering* (2025): 107458.
7. Khan, Mohammad Ilyas, Sarmina Samad, Ali Alamry, Talha Anwar, Ahmad Reza Norouzi, Hana Mohammed Mujlid, and S. P. Ghoushchi. "Enhancing Energy–Economic Performance and Environmental Sustainability of Parabolic Solar Collectors Using an Innovative Twisted Triangular Blades Turbulator." *Case Studies in Thermal Engineering* (2025): 107213.
8. Samad, Sarminah, Salman Saeidlou, M. Nadeem Khan, Ali Alamry, Laila M. Al-Harbi, Mohsen Sharifpur, and S. P. Ghoushchi. "Enhancing the hydrothermal and economic efficiency of parabolic solar collectors with innovative semi-corrugated absorber tubes, shell form cone turbulators, and nanofluid." *Case Studies in Thermal Engineering* (2025): 107003.
9. Ahmed, Abu Saleh, Md Shaharul Islam, M. A. M. A. Banggan, Emre Gorgun, M. Jameel, Alamry Ali, and Md Saiful Islam. "From Biomass to Biofuel: Innovative Microwave-Assisted Rapid Hydrothermal Liquefaction of Palm Kernel Shells." *International Journal of Chemical Engineering* 2025, no. 1 (2025): 9507978.
10. Manda, Muhamad Soffi Bin, Mohd Ruzaimi Mat Rejab, Shukur Abu Hassan, Mat Uzir Bin Wahit, Joseph Selvi Binoj, Brailson Mansingh Bright, Siti Safarah Binti Amirnuddin, Alamry Ali, and Kheng Lim Goh. "Effect of environmental exposure on long-term tensile strength of tin slag polymer concrete." *Next Sustainability* 5 (2025): 100139.
11. Rath, Debabrata, A. Alamry, Sudhir Kumar, Pratap Chandra Padhi, and Pratyush Pattnaāik. "Breaking boundaries: Optimizing dry machining for AISI D4 hardened tool steel through hybrid ceramic tool inserts." *Proceedings of the Institution of Mechanical Engineers, Part E: Journal of Process Mechanical Engineering* (2024): 09544089241265036.
12. Kumar, Sudhir, Inderjeet Singh, Alamry Ali, Shalok Bharti, Seyed Saeid Rahimian Koloor, and Geralt Siebert. "Science and engineering of composite materials: On in-house developed feedstock filament of polymer and polymeric composites and their recycling process–A comprehensive review." (2024).
13. Hammad, Ali S., Hong Lu, Mohamed M. El-Sayed Seleman, Mohamed MZ Ahmed, Ali Alamry, Jun Zhang, He Huang et al. "Impact of the tool shoulder diameter to pin diameter ratio and welding

speed on the performance of friction sir-welded AA7075-T651 Al alloy butt joints." *Materials Research Express* 11, no. 5 (2024): 056506.

14. Thooyavan, Yesudhasan, Lakshmi Annamali Kumaraswamidhas, Robinson Dhas Edwin Raj, Joseph Selvi Binoj, Bright Brailson Mansingh, Antony Sagai Francis Britto, and Alamry Ali. "Modelling and characterization of basalt/vinyl ester/SiC micro-and nano-hybrid biocomposites properties using novel ANN–GA approach." *Journal of Bionic Engineering* 21, no. 2 (2024): 938-952.
15. Ahmed, Mahmoud SI, Mohamed MZ Ahmed, Hussein M. Abd El-Aziz, Mohamed IA Habba, Ashraf F. Ismael, Mohamed M. El-Sayed Seleman, Ali Abd El-Aty et al. "Cladding of carbon steel with stainless steel using friction stir welding: effect of process parameters on microstructure and mechanical properties." *Crystals* 13, no. 11 (2023): 1559.
16. Alamry, Ali. "Fatigue damage and analysis of laminated composites: A state-of-the-art." *Journal of Engineering Research* (2024).
17. Ahmed, Abdalla, Alamry Ali, Bandar Alzahrani, and Kazuaki Sanada. "Evaluation of the viscoelastic behavior, thermal transitions, and self-healing efficiency of microcapsules-based composites with and without a catalyst using dynamic mechanical analysis technique." *Journal of Applied Polymer Science* 140, no. 34 (2023): e54323.
18. Abd El-Aty, Ali, Sangyul Ha, Yong Xu, Yong Hou, Shi-Hong Zhang, Bandar Alzahrani, Alamry Ali, and Mohamed MZ Ahmed. "Coupling computational homogenization with crystal plasticity modelling for predicting the warm deformation behaviour of AA2060-T8 Al-Li alloy." *Materials* 16, no. 11 (2023): 4069.
19. Ali, Alamry, Md Saiful Islam, Sinin Hamdan, and Masuk Abdullah. "Enhancing the performance of hybrid bio-composites reinforced with natural fibers by using coupling agents." *Materials Research Express* 12, no. 3 (2025): 035504.
20. Ahmed, Abdalla, Alamry Ali, Bandar Alzahrani, and Kazuaki Sanada. "Investigating the influence of self-healing microcapsule volume fraction on the dynamic mechanical properties and self-healing performance of epoxy-based composites." *Journal of Polymer Research* 31, no. 7 (2024): 201.
21. Abd El-Aty, Ali, Cheng Cheng, Yong Xu, Yong Hou, Jie Tao, Shenghan Hu, Bandar Alzahrani, Alamry Ali, Mohamed MZ Ahmed, and Xunzhong Guo. "Modeling and experimental investigation of UR relationship of AA6061-T6 tubes manufactured via free bending forming process." *Materials* 16, no. 23 (2023): 7385.

22. Ahmed, Abu Saleh, Alamry Ali, Emre Gorgun, M. Jameel, Tasmina Khandaker, Md Shaharul Islam, Md Saiful Islam, and Masuk Abdullah. "Microalgae to Biofuel: Cutting-Edge Harvesting and Extraction Methods for Sustainable Energy Solution." *Energy Science & Engineering* (2025).
23. Mansingh, Bright Brailson, Joseph Selvi Binoj, Shukur Abu Hassan, Gudaru Kumar Raja, Alamry Ali, and Kheng Lim Goh. "Bio-fillers: physicochemical nature, properties, and resources." In *Sustainable Fillers/Plasticizers for Polymer Composites*, pp. 57-75. Elsevier Science Ltd, 2025.
24. Kumar, Sudhir, Inderjeet Singh, Alamry Ali, Shalok Bharti, Seyed Saeid Rahimian Koloor, and Geralt Siebert. "On in-house developed feedstock filament of polymer and polymeric composites and their recycling process–A comprehensive review." *Science and Engineering of Composite Materials* 31, no. 1 (2024): 20220238.
25. Ali, Alamry, Seyed Saeid Rahimian Koloor, Abdullah H. Alshehri, and A. Arockiarajan. "Carbon nanotube characteristics and enhancement effects on the mechanical features of polymer-based materials and structures–A review." *Journal of Materials Research and Technology* 24 (2023): 6495-6521.
26. Ali, Alamry, and Andri Andriyana. "Properties of multifunctional composite materials based on nanomaterials: a review." *RSC advances* 10, no. 28 (2020): 16390-16403.
27. Gorgun, Emre, Alamry Ali, and Md Saiful Islam. "Biocomposites of poly (lactic acid) and microcrystalline cellulose: influence of the coupling agent on thermomechanical and absorption characteristics." *ACS omega* 9, no. 10 (2024): 11523-11533.
28. Meraz, Md Montaseer, Md Habibur Rahman Sobuz, Nusrat Jahan Mim, Alamry Ali, Md Saiful Islam, Md Abu Safayet, and Md Tanjid Mehedi. "Using rice husk ash to imitate the properties of silica fume in high-performance fiber-reinforced concrete (HPFRC): A comprehensive durability and life-cycle evaluation." *Journal of Building Engineering* 76 (2023): 107219.
29. Essa, Ahmed RS, Ramy IA Eldersy, Mohamed MZ Ahmed, Ali Abd El-Aty, Ali Alamry, Bandar Alzahrani, Ahmed E. El-Nikhaily, and Mohamed IA Habba. "Modeling and experimental investigation of the impact of the hemispherical tool on heat generation and tensile properties of dissimilar friction stir welded AA5083 and AA7075 Al alloys." *Materials* 17, no. 2 (2024): 433.
30. Ali, Alamry, Andri Andriyana, Shukur Bin Abu Hassan, and Bee Chin Ang. "Fabrication and thermo-electro and mechanical properties evaluation of helical multiwall carbon nanotube-carbon fiber/epoxy composite laminates." *Polymers* 13, no. 9 (2021): 1437.
31. Alshehri, Abdullah H., Ali Alamry, Seyed Saeid Rahimian Koloor, Bandar Alzahrani, and A. Arockiarajan. "Investigating low velocity impact and compression after impact behaviors of carbon fiber/epoxy composites reinforced with helical multiwalled carbon nanotubes." *Journal of Engineering Research* (2024).

32. El-Aty, Ali Abd, Yong Xu, Wenlong Xie, Liang-Liang Xia, Yong Hou, Shihong Zhang, Mohamed MZ Ahmed et al. "Finite element analysis and experimental study of manufacturing thin-walled five-branched AISI 304 stainless steel tubes with different diameters using a hydroforming process." *Materials* 17, no. 1 (2023): 104.
33. Dubi, Y., & Di Ventra, M. (2017). Colloquium: Heat flow and thermoelectricity in atomic and molecular junctions. *Reviews of Modern Physics*, 83(1), 131–155. https://doi.org/10.1103/RevModPhys.83.131
34. Liu, J., Sun, Q., & Xie, Z. (2018). Enhanced thermoelectric efficiency in molecular wire systems via quantum interference effects. *Physical Chemistry Chemical Physics*, 20(12), 8121–8128. https://doi.org/10.1039/C7CP08534A
35. Finch, C. M., García-Suárez, V. M., & Lambert, C. J. (2016). Giant thermopower and figure of merit in single-molecule devices. *Physical Review B*, 79(3), 033405. https://doi.org/10.1103/PhysRevB.79.033405
36. Kim, Y., Jeong, W., Kim, K., Lee, W., & Reddy, P. (2019). Electrostatic control of thermoelectricity in molecular junctions. *Nature Nanotechnology*, 9(11), 881–885. https://doi.org/10.1038/nnano.2014.209