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Unveiling Process–Structure–Property Coupling in CNT Fibers via Multimodal AI Analytics

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Carbon nanotubes (CNTs) exhibit an exceptional combination of low density, outstanding mechanical properties, and high electrical and thermal conductivity, making them attractive for structural and functional applications. To translate these nanoscale properties into practical materials, extensive efforts have been devoted to assembling CNTs into macroscopic fibers. However, a central challenge in CNT fiber research lies in the pronounced gap between the intrinsic properties of individual CNTs and the macroscopic performance of CNT fibers, indicating that the superior properties of CNTs are not yet fully exploited.

CNT fibers are governed by numerous processing parameters, including dispersion, spinning, and post-treatment conditions, as well as by multiscale structural factors such as CNT structure, bundle and aggregation states, and overall fiber architecture. These factors are highly coupled, resulting in a complex, high-dimensional process–structure–property relationship that cannot be adequately understood using conventional one-parameter or empirical approaches. A similar challenge was historically encountered in carbon fiber development, which required several decades—from its emergence in the 1950s to large-scale adoption in aircraft such as the Boeing 777 and 787—to achieve sufficient understanding and optimization [1]. This historical perspective highlights the need for accelerated research strategies, including the adoption of artificial intelligence (AI)-assisted approaches. In this study, an AI-based analytical approach is introduced to aid in understanding this complex process–structure–property relationship and to explore its application to mechanism elucidation.

Aqueous CNT dispersions stabilized with surfactants were prepared as spinning dopes, and continuous CNT fibers were fabricated by wet spinning. Structural characteristics were evaluated across different process stages, including aggregation states in the liquid dispersions and defect formation and bundle assembly in the resulting fibers, encompassing multiscale and multidimensional features inherent to CNT fiber processing. Mechanical and electrical properties, including tensile strength, Young's modulus, and electrical conductivity, were also measured.

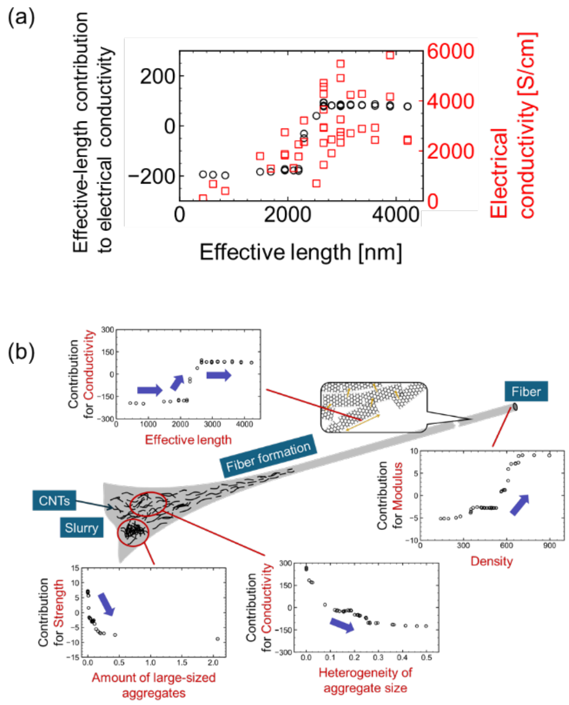

Fig. 1: (a) Representative example of structure–property relationships, shown as the relationship between CNT effective length and electrical conductivity, together with its contribution obtained from AI-based analysis. (b) Schematic illustration of the relationships between multiscale structural features of CNT fibers and aqueous spinning dopes and the resulting properties. The multiscale structures influence tensile strength, electrical conductivity, and Young's modulus.

For distribution-type structural data that are difficult to interpret using conventional physical descriptors, non-negative matrix factorization (NMF) was employed to extract representative features. These features were integrated with additional structural descriptors, such as density and the CNT G/D ratio, as well as processing parameters, to construct property prediction models targeting multiple properties. The trained models were further analyzed using

SHAP to assess the relative importance and contributions of individual features to the predicted properties. Detailed experimental conditions and analytical procedures are described in our previous publications [2, 3].

AI-assisted analysis clarified the independent contributions of individual structural factors that could not be captured by simple structure–property correlations, revealing nonlinear relationships between structure and properties (Figure 1). In particular, nanoscale CNT defect descriptors, such as the G/D ratio and effective length, were found to influence tensile strength, Young's modulus, and electrical conductivity in different ways. In addition, the effects of aggregate size and uniformity in the dispersions on the resulting properties also varied depending on the targeted property.

These findings provide insights into the mechanisms governing property enhancement, including the role of macroscopic defects in tensile strength and the influence of nanoscale CNT defects and conductive path formation on electrical conductivity. Furthermore, threshold values of key structural factors were identified, leading to practical design guidelines; for example, electrical conductivity was enhanced when mild dispersion conditions were employed to maintain the CNT effective length at approximately 2000 nm. Overall, this study demonstrates that explainable, multimodal AI-based analysis is a powerful approach for elucidating mechanisms and accelerating research in complex material processing systems.

References

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