Experiment–Machine Learning Synergy for Catalytic Carbonization of Polyetherimide/Graphite Nanocomposites

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Abstract

Polyetherimide (PEI) is an attractive polymer precursor for producing high-performance carbonaceous materials for applications ranging from gas separation membranes and energy storage to thermal insulation and structural foams. In our recent study, we systematically investigated the catalytic pyrolysis of PEI/graphite (Gr) nanocomposites with Fe, Co, and Ni catalysts using thermogravimetric analysis (TGA) under nitrogen. Response surface methodology revealed that char yield is maximized for Fe- and Co-containing nanocomposites at 100 phr Gr and 10 °C/min heating rate, achieving ~55–57% improvement over neat PEI. Structural characterization (Raman, XRD, XPS) showed that Co promoted graphitization while Fe induced defect-rich carbons through Fe–N and Fe–C interactions, validating the catalytic role in tailoring microstructure [1]. Building upon this experimental dataset, we developed a physics-informed, transformer-based machine learning (ML) model to predict the thermal decomposition and char mass evolution of PEI/Gr nanocomposites. The model incorporated catalyst properties (e.g., d-orbital electrons, carbide formation energies), graphite structural parameters, and kinetic features derived from Avrami–Erofeev models. Trained on Fe and Ni systems and tested on unseen Co formulations, the ML framework achieved $R^2 > 0.98$, accurately capturing TGA curves and kinetic trends. Importantly, the model generalized beyond training conditions, offering predictive insights into catalytic effects on pyrolysis. Together, these complementary experimental and ML approaches establish a robust framework for designing carbon nanocomposites with tailored char yield, graphitization degree, and functional performance. This synergy between transition metal catalysis and data-driven modeling provides new opportunities for scalable development of carbon-based membranes, foams, and energy storage systems.

References

[1] Salavati, M.; Majdoub, M.; Oulhakem, O.; Sengottuvelu, D.; Villacorta, B. S.; Ucak-Astarlioglu, M. G.; Al-Ostaz, A.; Nouranian, S. *ACS Appl. Nano Mater.* 2025, 8, 30, 15060–15074

Figures

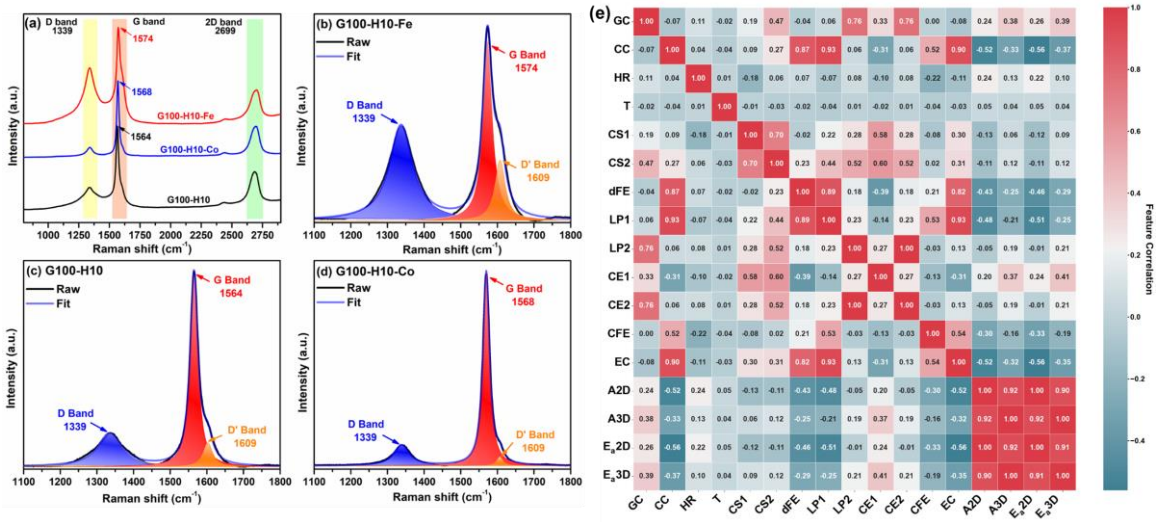

Figure 1: (a) Raman spectra, (b-d) Raman deconvolution, and (e) XRD patterns of PEI/Gr/catalysts;(e) Feature correlation heatmap for graphite content (GC), catalyst content (CC), heating rate (HR), temperature (T), catalyst (1) and Gr (2) crystal systems (CS1 and CS2), d-orbital free electrons (dFE), lattice parameter (LP1 and LP2), cohesive energy (CE1 and CE2), carbide formation energy (CFE), electrical conductivity (EC), pre-exponential factors for 2D and 3D kinetic models (A2D and A3D), and activation energies (Ea_2D and Ea_3D).