Chemistry and Properties of Carbon Fiber Feedstocks from Bitumen Asphaltenes

Martha L. Chacón-Patiño,[1] Anika Neumann,[2] Christopher P. Rüger,[2] Paolo G. Bomben,[3] Lukas Friederici,[2] Ralf Zimmermann,[2] Erik Frank,[4] Philipp Kreis,[4] Michael R. Buchmeiser,[4] and Murray R. Gray[3]

1. National High Magnetic Field Laboratory; 2. Joint Mass Spectrometry Centre, University of Rostock, Germany; 3. Alberta Innovates, Canada; 4. German Institutes of Textile- and Fiber Research, Denkendorf, Germany

Funding Grants: G.S. Boebinger (NSF DMR-1644779 & DMR-2128556); Zimmermann (EU_FT-ICR MS, 731077, and DFG INST 264/56)

Carbon fibers are essential for many applications, including aerospace and medical devices. Most fibers are made from polyacrylonitrile, which is quite expensive. Carbon fiber manufacturing from low-value petroleum feedstocks, which are highly enriched in asphaltenes, could decrease precursor costs by as much as 90%, and reduce greenhouse gas emissions. Asphaltenes are comprised of polycyclic aromatic hydrocarbons (PAH) organized into two structural motifs, as shown in **Figure 1**. "Single-core" PAH are fused into a single planar unit, whereas "multicore" compounds contain several smaller PAH units linked by flexible covalent bonds. Successful transformation of asphaltenes into carbon fibers requires a detailed understanding of how thermal treatment affects their composition and fiber stability. For example, sulfur-containing PAH (PASH) releases carbon disulfide bubbles within the fibers, diminishing fiber performance.

In this work, MagLab users investigated correlations between carbon fiber production processes and asphaltene composition. Asphaltene-enriched feedstocks were thermally treated under different conditions to direct their chemistry. Samples were characterized by 21T FT-ICR MS and gas-phase fragmentation (MS/MS spectra, **Figure 1**). The results indicate that severe thermal treatment yielded bad source material molecules (* **Figure 1 upper right**), which in MS/MS revealed building blocks (blue arrow) consistent with single-core, high-molecular-weight PAH/PASH. No stable carbon fibers could be produced from these samples. Conversely, a feedstock treated with mild thermal conditions in molten sodium, a process designed to remove sulfur, yielded good source material molecules (* **Figure 1 lower right**). Those compounds contained abundant multi-core structural motifs, as shown by the abundant presence of low-molecular-weight PAH (yellow dashed line). These materials produced stable carbon fibers. Thus, the investigation of complex asphaltene composition by 21T FT-ICR MS with gas-phase fragmentation guides feedstock upgrading into effective carbon fiber precursors.

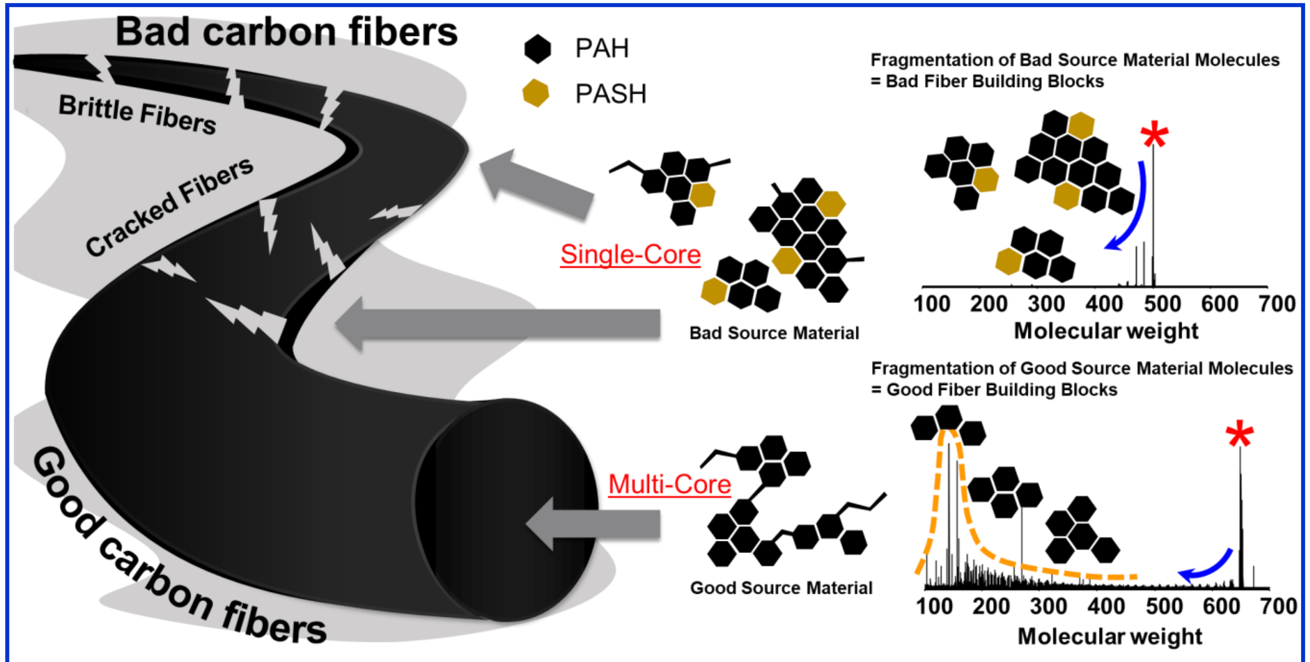

Figure 1. Gas-phase fragmentation mass spectra (MS/MS) for bad (top right) and good (bottom right) source materials for carbon fiber production. Bad source material molecules contain abundant single-core molecules comprised of high-molecular-weight PAH and PASH, which produce no stable carbon fibers upon spinning. Conversely, good source material molecules contain abundant multicore compounds composed of low molecular weight, interconnected PAH and produce good carbon fibers. Bad source materials are identified in FT-ICR mass spectra by production of high mass fragments (upper right, blue arrow). Good source materials are identified by production of low mass fragments (bottom right, yellow dashed line).

Facilities and instrumentation used: ICR User Facility, 21T FT-ICR Mass spectrometer

Citation: Chacon Patino, M.L.; Neumann, A.; Ruger, C.P.; Bomben, P.G.; Friederici, L.; Zimmerman, R.; Frank, E.; Kreis, P.; Buchmeiser, M.R.; Gray, M.R., *Chemistry and Properties of Carbon Fiber Feedstocks from Bitumen Asphaltenes*, **Energy Fuels**, **37** (7), 5341-5360 (2023) doi.org/10.1021/acs.energyfuels.2c04274 - Data Set