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Microstructure defines the electroconductive and mechanical performance of plant-derived renewable carbon fiber

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Introduction

- Lignin as a major by-product from paper industry and biorefinery can be an alternative precursor of polyacrylonitrile (PAN) for renewable and low-cost carbon fiber. With a high electroconductive and mechanical performances, lignin based carbon fiber can be applied not only as structure composite materials, but also in battery electrode materials.
- This study revealed that both the electroconductive and mechanical performances of lignin-based CF were synergistically improved by enhancing the microstructures through modifying the lignin chemistry.

Materials and Methods

- 2 fraction of Kraft lignin was used to create experimental group with different molecule weight, PDI, G/D ratio and inter-linkage content. Eight sorghum variants was extracted using a organosolv method for a more rigorous verification. [1][2]
- Lignin-based carbon fibers were prepared by a wet-spinning set-up (Fig1) followed by thermostabilization and carbonization
- The microstructures of lignin-based carbon fiber were analyzed by both X-ray diffraction (XRD) and Raman microscopy. The crystallite size was calculated from this (002) peak using Scherrer's equation. Lignin interlinkage was analyzed by 2D HSQC NMR.

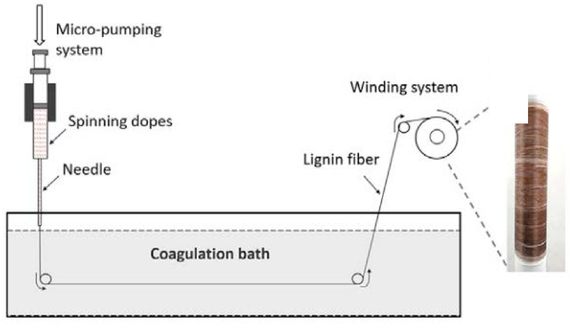

Fig 1. The fabrication process of lignin carbon fiber

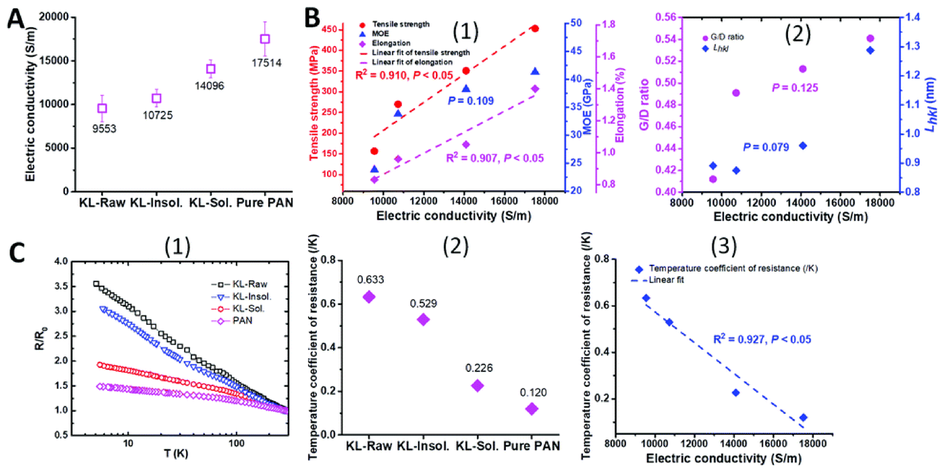

Fig 2. Microstructures as characterized by XRD (A) and Raman spectroscopy (B), and mechanical properties (C) and their linear correlation with crystallite structures (D)

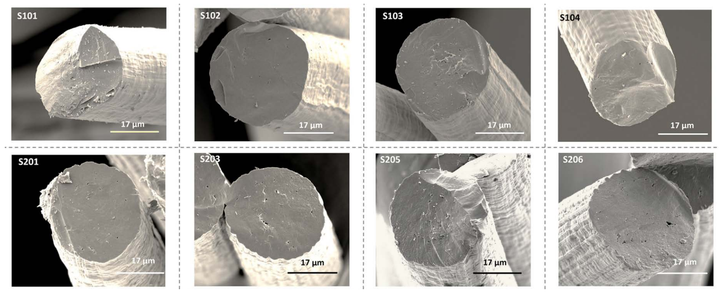

Fig 3. SEM images of the cross sections of the resultant carbon fibers

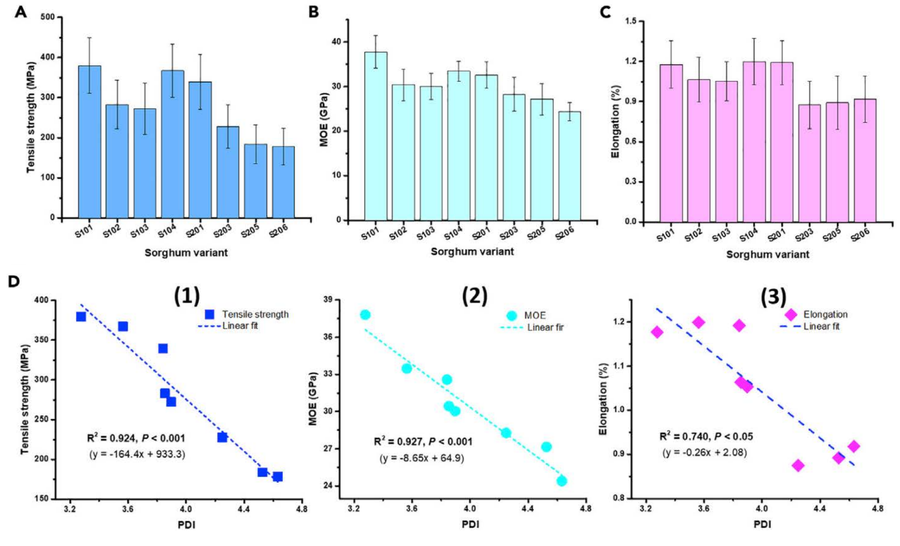

Fig 4. The Mechanical Properties of Lignin-based Carbon Fibers and their Correlation Relationships with Biomass Characteristics

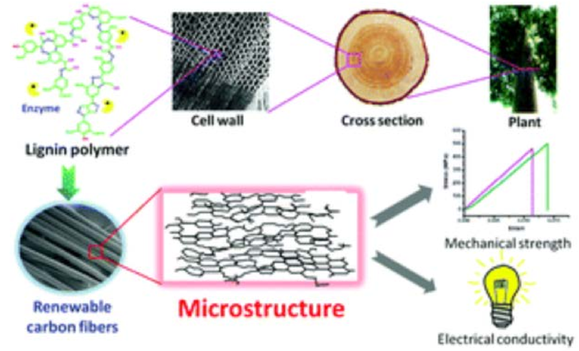

Fig 4. Concept of Valorizing Lignin from Biomass as an Alternative Precursor of Polyacrylonitrile to Make Carbon Fiber

Results

- MOE, tensile strength and elongation, were increased from 23.9 GPa, 157 MPa and 0.83% for carbon fiber made of raw Kraft lignin/PAN to 33.6 GPa, 270 MPa and 0.96% for carbon fiber made of water-insoluble lignin/PAN, and further increased to 38.2 GPa, 351 MPa and 1.05% for carbon fiber made of water-soluble lignin/PAN, respectively.(Fig 2)
- Linear correlations between PDI and tensile strength (R2 = 0.924, P < 0.001), MOE (R2 = 0.927, P < 0.001), and elongation (R2 = 0.740, P < 0.05) is as shown in Fig 4. Lignin content, composition (S/G ratio), molecular weight were not found linear correlations with mechanical performance(data is not shown).

Conclusion

- All microstructure characteristics of Lhkl, dhkl, and G/D ratio had significant linear correlations with mechanical performance properties (Figures 4F–4H), indicating that crystallite size (Lhkl), crystallite content (G/D ratio), and the distances between crystallite layers (dhkl) all impact on the carbon fiber performances
- Electroconductive and mechanical performances are higlly related to the fiber microstructure
- The molecular uniformity of lignin polymer was revealed as a critical determinant defining the quality of the resultant lignin-based carbon fibers. The study indicated that further research to design feedstock, and reconfigure biomass processing will be needed to manufacture value-added lignin materials.

Literature Cited

✓[1] Qiang Li,et al. Discovering Biomass Structural Determinants Defining the Properties of Plant-Derived Renewable Carbon Fiber. iScience 23, 101405(2020).

✓[2] Qiang Li,et al. Microstructure defines the electroconductive and mechanical performance of plant-derived renewable carbon fiber. Chemical Communications 55, 12655-12658(2019).