**Experimental and Simulative Investigations of Polymer Derived Carbon with Boron Nitride Nanotube Reinforcements**

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**Abstract**

Carbon-fiber reinforced carbon matrix composites have gained considerable attention due to their superior properties, including a high stiffness-to-weight ratio, excellent thermal and electrical conductivity, and a low coefficient of thermal expansion. These attributes make them ideal for demanding applications in aerospace, defense, and high-temperature environments. Recent studies have shown that substituting carbon fibers with carbon nanotubes (CNTs) as primary reinforcements in carbon matrices can significantly enhance composite performance, largely due to the nanoscale dimensions and high aspect ratio of CNTs. Boron nitride nanotubes (BNNTs), which are structural analogues of CNTs, offer additional advantages. Their polar B–N bonds potentially enable improved interfacial bonding with the matrices, and they exhibit superior thermal stability under oxidative conditions. This dissertation investigates the structure evolution and mechanical behaviors of BNNT-reinforced carbon matrix composites, focusing on their processing and structure-property relationships.

Thin films were fabricated by dispersing varying weight fractions of BNNTs in phenolic resin. The suspensions were drop-cast, dried, cured, and subsequently pyrolyzed at two temperatures: 1200 °C and 1500 °C. Structural characterization was conducted using Raman spectroscopy and X-ray diffraction (XRD) to assess the impact of BNNTs on the carbon matrix's crystallinity. Raman results revealed a decrease in the ID/IG ratio with increasing BNNT content, indicating enhanced graphitic ordering. XRD analysis confirmed that higher BNNT loadings led to interlayer spacings approaching the graphitic d₀₀₂ value, suggesting improved stacking of turbostratic carbon layers. This templating effect is attributed to the presence of BNNTs within the matrix.

Mechanical testing of the pyrolyzed films demonstrated substantial improvements in strength and toughness. At 1200 °C, both fracture stress and strain increased with BNNT content, highlighting the beneficial role of BNNTs in load transfer and crack bridging. At 1500 °C, fracture stress continued to rise while fracture strain declined, indicative of increased stiffness due to graphitization. At 5 wt% BNNT loading, flexural strength, modulus, and toughness improved by 68.7%, 55.6%, and 87.8%, respectively. These properties exhibited nearly an order-of-magnitude enhancement at 1500 °C, further supported by evidence of new interfacial bond formation that strengthened with increasing temperature.

To complement the experimental findings, finite element modeling (FEM) was performed to estimate the effective elastic properties of the BNNT-reinforced carbon matrix composites. Representative volume elements (RVEs) were constructed using periodic boundary conditions and homogenization theory to simulate the composite’s macroscopic response. The simulations accounted for constituent properties, as well as the shape and spatial distribution of BNNTs. The resulting predictions were validated against analytical models, including the Rule of Mixtures and Halpin-Tsai equations, both of which showed good agreement with the FEM-derived values.

This work establishes BNNTs as effective nanoscale reinforcements in carbon matrix composites, offering improved structural ordering, and mechanical performance—critical for their deployment in next-generation high-temperature structural applications.