Influence of CNT Orientation on the Mechanical Properties of SiC/CNT Composites: A Molecular Dynamics Study

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Carbon nanotube (CNT) are known to enhance the toughness and strength of SiC ceramic matrices, but their reinforcement capability is constrained by atomic-scale structural factors, particularly CNT orientation[1]. The specific ways in which orientation influences reinforcement are not yet fully understood. In this study, bond-order-based reactive molecular dynamics simulations are used to explore the mechanical properties and deformation mechanisms of SiC/CNT composites with varying CNT orientations.

As a resuly, this study elucidates two reinforcement mechanisms based on CNT orientation: "axial stretching," where CNTs are stretched to bear the composite load, and "crack bridging," where CNTs link grains like a bridge. The results indicate that as the angle (θ) between CNTs and the tensile direction increases, axial stretching intensifies, while CNT bridging weakens. This leads to a decrease in composite strength due to the increased reliance on CNT axial stretching. Meanwhile, toughness exhibits a volcano-shaped trend, driven by the competing effects of both mechanisms. By accounting for factors such as SiC crystalline structure, CNT wall number, diameter, aspect ratio, and defects, the study introduces a modified, generalized rule of mixtures. This approach equates the CNT orientation correction factor to the cosine of θ, facilitating the theoretical prediction of tensile strength in fiber-reinforced ceramic matrix composites.

References

1. Joshi, U. A.; Sharma, S. C.; Harsha, S. P. *Compsites: Part B*, **2021**, *43*, 2063 – 2071.