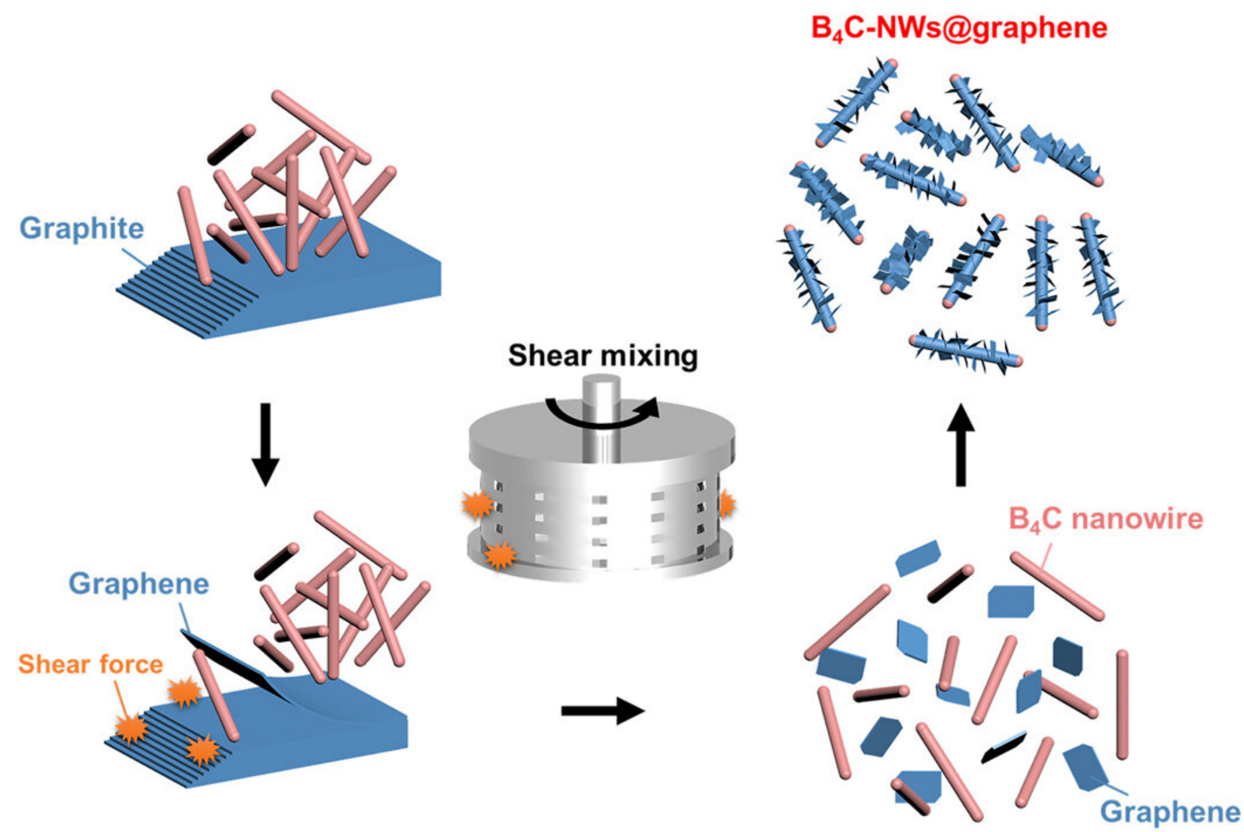
Tailoring nanocomposite interfaces with graphene to achieve high strength and toughness

October 27 2020, by Thamarasee Jeewandara

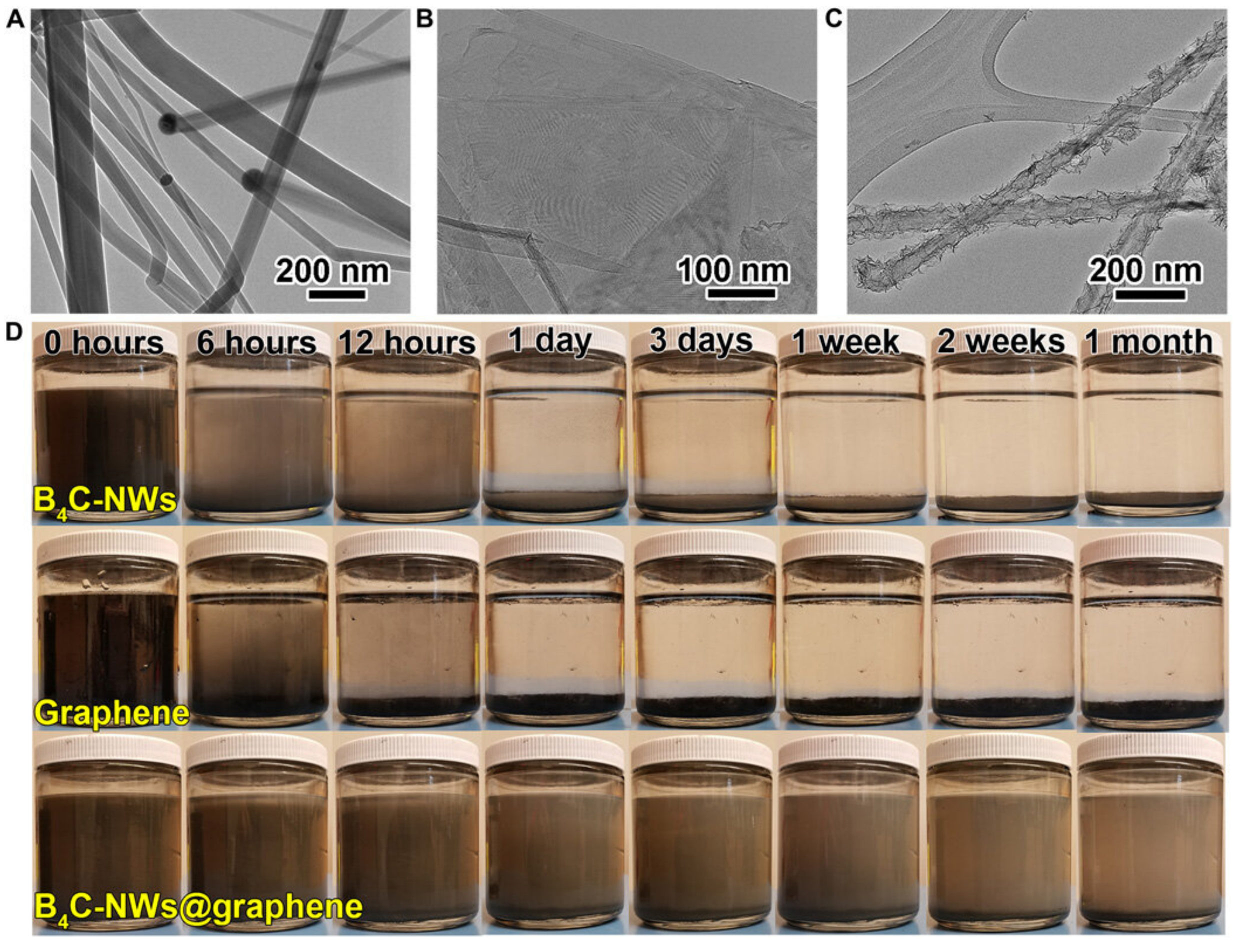


Schematic illustration of the synthesis process steps of B4C-NWs@graphene formation. Credit: Science Advances, doi: 10.1126/sciadv.aba7016

The weak interfacial interaction between nanofillers and matrix nanocomposites during materials engineering have caused nanofiller reinforcing effects to be far below the theoretically predicted values. In a new report now published on *Science Advances*, Ningning Song, and a team of scientists at the department of mechanical and aerospace engineering at the University of Virginia, U.S., demonstrated graphene-wrapped boron carbide (B_4C) nanowires (B_4C-NWs@graphene). The constructs empowered exceptional dispersion of nanowires in the matrix and contributed to superlative nanowire-matrix bonding. The B_4C-NWs@graphene constructs reinforced epoxy composites and showed simultaneous enhancement in strength, elastic modulus and ductility. By using graphene to tailor the composite interfaces, Song et al. effectively used the nanofillers to increase the load transfer efficiency by two-fold. They used molecular dynamics simulations to unlock the shear mixing self-assembly mechanism of the graphene/nanowire construct. The low-cost technique opens a new path to develop strong and tough nanocomposites to improve interfaces and allow efficient high load transfer.

Nanofillers – nanowires and nanoparticles

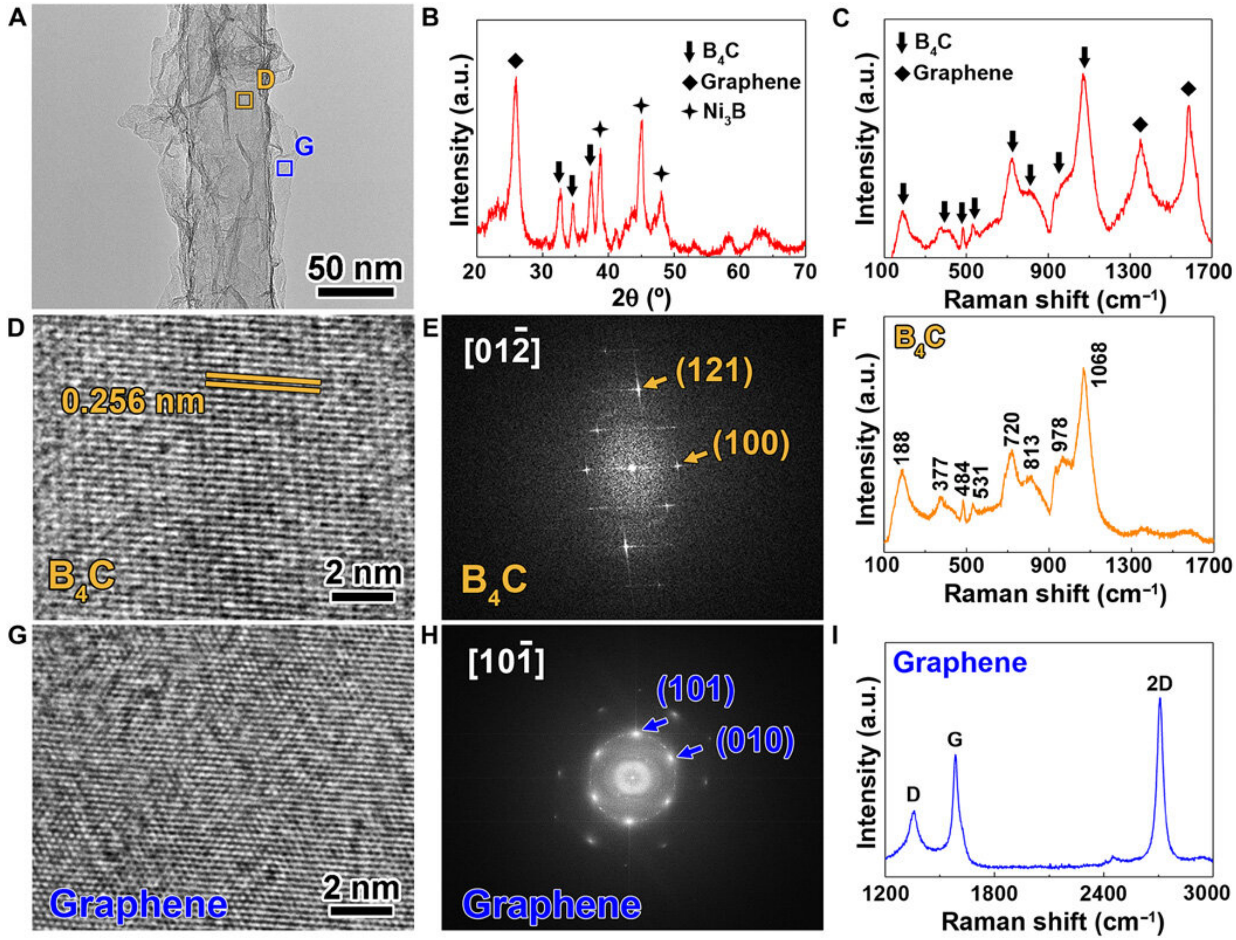
Nanofillers including nanowires and nanoparticles can have much larger specific surface areas than microfillers. In theory, they therefore offer ideal reinforcements for exceptional joint enhancements in strength and toughness. However, in materials science and engineering, nanocomposites remain to fulfill this promise due to the weak interfacial bonding between the fillers and the matrix. Boron carbide (B_4C) is the third hardest material known in nature, often acclaimed for its key physical and mechanical properties. However, when employed as reinforcements in nanocomposites, the B_4C nanowires (B_4C-NWs) alone do not show a reinforcing effect due to its weak dispersion in the matrix and due to weak interfacial bonding. As a result, it is important to engineer nanocomposite interfaces to realize their full potential. Of the many approaches at play and previously explored in materials science and nanomaterials, Song et al. report a graphene interface engineering technique. In this mechanism, they glued B_4C-NWs with graphene to exceptionally enhance the strength and toughness of the resulting material. They converted the high-quality graphene sheets to graphite and simultaneously wrapped them on to the B_4C-NWs via shear mixing to obtain the B_4C-NWs@graphene constructs.



Synthesis of nanofillers in dilute water by shear mixing. TEM images of (A) B4C-NWs, (B) multilayered graphene, and (C) B4C-NWs@graphene. (D) Chronological digital photos of the suspensions of B4C-NWs, graphene, and B4C-NWs@graphene. Photo credit: Ningning Song, University of Virginia. Credit: Science Advances, doi: 10.1126/sciadv.aba7016

Synthesizing the B_4C-NWS@graphene constructs

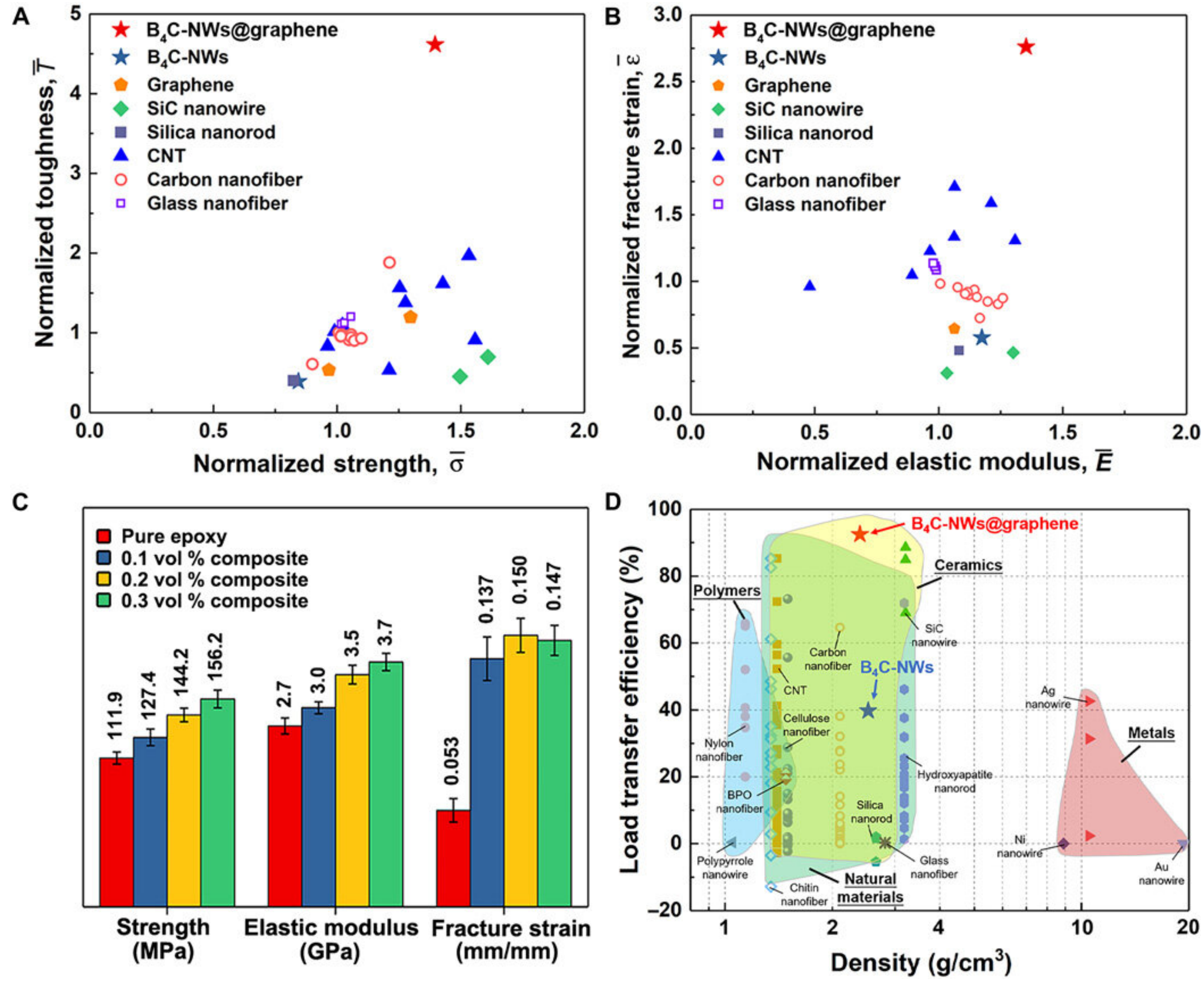
Song et al. first grew B_4C-NWS uniformly on the surface of a carbon fiber cloth through a typical vapor-liquid-solid process, where cotton served as a source of carbon, while amorphous boron powders served as a source of boron, alongside a catalyst. The team separated the B_4C-NWS from the substrate via ultrasonic vibrations and studied the chemical bonding states in the material using X-ray photoelectron spectroscopy (XPS) to confirm the production of high-quality B_4C-NWs. To then directly synthesize and self-assemble the B_4C-NWs@graphene, Song et al. mixed graphite powders and B_4C-NWs. Then using transmission electron microscopy (TEM), they showed how graphite was successfully exfoliated to graphene, while B_4C-NWS remained intact in the mixture. During the synthetic procedure, the graphene sheets simultaneously self-assembled onto the B_4C-NWs surface. Using both high-resolution transmission electron microscopy (HRTEM) inspection and the corresponding fast Fourier transform (FFT) pattern, Song et al. confirmed self-assembly of graphene on the B_4C-NWs with high quality, while maintaining monolayered and multi-layered features.



Characterization of B4C-NWs@graphene. (A) TEM image, (B) XRD pattern, and (C) background-corrected Raman spectrum of B4C-NWs@graphene. (D) HRTEM image, (E) the corresponding FFT, and (F) background-corrected Raman spectrum of the B4C-NWs in B4C-NWs@graphene. (G) HRTEM image, (H) the corresponding FFT, and (I) background-corrected Raman spectrum of the monolayered graphene in B4C-NWs@graphene. a.u., arbitrary units. Credit: Science Advances, doi: 10.1126/sciadv.aba7016

Characterizing the B_4C-NWs@graphene constructs

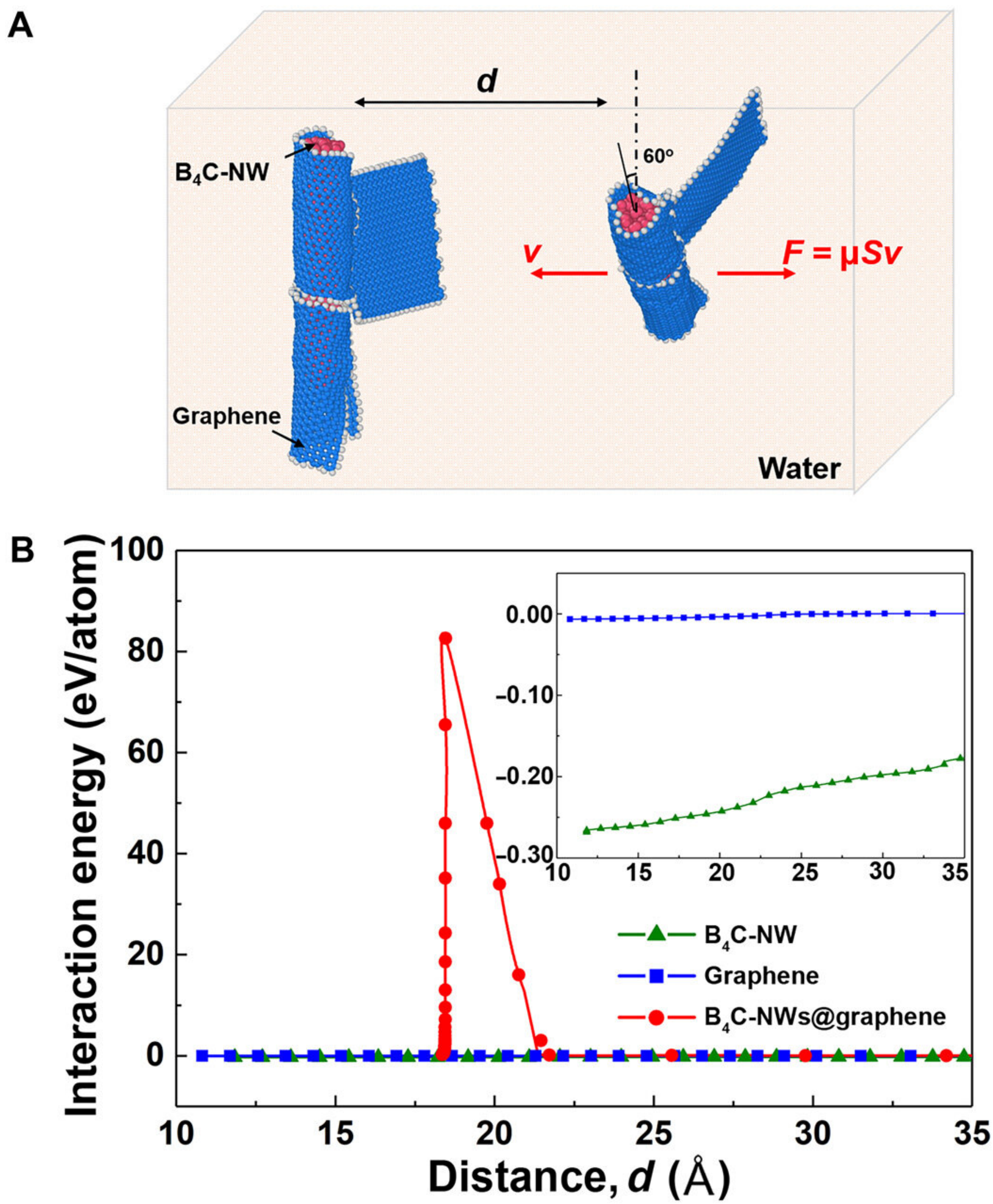
The scientists dispersed the B4C-NWs@graphene on to epoxy nanocomposites and conducted three-point bending tests on the composites and epoxy materials. Compared to raw epoxy resin samples, the B_4C-NWs@graphene nanocomposites underwent a larger plastic deformation before fracture. The results showed how graphene strengthened the bond between the B_4C-NWs and the epoxy matrix as an interfacial agent, while a series of mechanism that facilitated bending jointly contributed to enhanced toughness of the B_4C-NWs@graphene composites. In this way, graphene allowed better dispersion capabilities for the nanofillers in the matrix, providing improved load transfer and joint amplification in strength and toughness. To better understand the dispersion quality of B_4C-NWs@graphene constructs, Song et al. calculated the theoretical elastic modulus of the composites. The results showed that the composites retained exceptional strength and toughness when compared with other composites reported in literature.



Mechanical performance of B4C-NWs@graphene composites.(A and B) Comparison of mechanical properties of 0.3 vol % B4C-NWs@graphene composites with other typical nanofiller reinforced composites [derived from (30–44)]. (C) Comparison of flexural strength, elastic modulus, and fracture strain for pure epoxy and B4C-NWs@graphene reinforced composites. (D) Load transfer efficiency versus density chart showing that the B4C-NWs@graphene composite had exceptional interface properties [mechanical properties of 1D nanofiller reinforced composites were derived from previous studies]. CNT, carbon nanotube. Credit: Science Advances, doi: 10.1126/sciadv.aba7016

Molecular dynamics simulations

The team conducted molecular dynamics (MD) simulations to first understand how graphene sheets edited the B_4C-NW surface and how graphene allowed the dispersion of B_4C-NWs as well as enhanced load transfer in the composites. They then performed MD simulations to test the pull-out process of nanofillers from an epoxy matrix to understand the adhesive strength between the nanofillers and the matrix. The MD simulations agreed with the experimental observations and uncovered details of the enhanced interaction barrier of the graphene-tailored B_4C-NWs to improve dispersion performance. Song et al. performed simulations to investigate the pull-out process of nanofillers from the epoxy matrix and calculated the interaction energy to understand the adhesive strength between the nanofillers and the matrix. The B_4C-NWs@graphene showed higher interaction energy with epoxy and larger pull-out peak force due to the presence of graphene, which rendered the nanofiller with higher surface area. In addition, the larger number of interacting atoms and complex geometries of the composite enhanced the interfacial strength and load transfer efficiency.



The MD simulations of the nanofiller interactions. (A) MD snapshots of the initial structure (B4C-NWs@graphene/B4C-NWs@graphene) for calculating the interaction energy. (B) Interaction energy profiles between two nanofillers of the same type (graphene/graphene, B4C-NW/B4C-NW, and B4C-NWs@graphene/B4C-NWs@graphene). Credit: Science Advances, doi: 10.1126/sciadv.aba7016

In this way, Ningning Song and colleagues used graphene sheets to tailor the interface between B_4C-NWs and epoxy materials. The team synthesized the nanocomposite material (B_4C-NWs@graphene) by shear mixing graphene powders and B_4C-NWs in dilute water. The resulting suspension showed homogenous dispersion in water and in epoxy materials for enhanced load transfer efficiency, while improving the mechanical performance of the composites. This low-cost and efficient graphene-wrapping technique will open new paths to develop strong and tough nanocomposites, with applications in medicine, pharmacology and drug delivery, allowing graphene wrapped nanoparticles to overcome efflux pumps and drug resistance.

More information: Ningning Song et al. Tailoring nanocomposite interfaces with graphene to achieve high strength and toughness, *Science Advances* (2020). DOI: 10.1126/sciadv.aba7016

A. K. Geim et al. The rise of graphene, *Nature Materials* (2007). DOI: 10.1038/nmat1849

Ian A. Kinloch et al. Composites with carbon nanotubes and graphene: An outlook, *Science* (2018). DOI: 10.1126/science.aat7439