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Synergistic Enhancement of Mechanical, Tribological, and Thermal Properties of UHMWPE Nanocomposites Through Hybrid MXene ($Ti_3C_2T_x$) and Hexagonal Boron Nitride Reinforcement: An Experimental Investigation

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Abstract

Ultra-High Molecular Weight Polyethylene (UHMWPE) occupies a unique position in engineering polymer science by virtue of its exceptional abrasion resistance, chemical inertness, and biocompatibility, yet its thermal conductivity (0.40–0.44 W/m·K) and moderate tensile strength (25–35 MPa) constrain its deployment in thermally demanding tribological applications such as orthopaedic bearing surfaces, industrial seal components, and high-load conveyor liners. This study presents a systematic experimental investigation of eight nanocomposite formulations incorporating two-dimensional MXene nanosheets ($Ti_3C_2T_x$, 1–5 wt%), hexagonal boron nitride (h-BN, 5–10 wt%), and dual hybrid combinations (MX3-BN5 and MX5-BN5), processed via bath sonication and dual-step ball-milling routes followed by uniaxial hot compression moulding at 180°C. Characterisation encompasses X-ray diffraction (XRD), Raman spectroscopy, Fourier-transform infrared spectroscopy (FTIR), and field-emission scanning electron microscopy with energy-dispersive X-ray analysis (FESEM-EDX) for microstructural evaluation; uniaxial tensile testing, Shore D hardness, and pin-on-disc tribometry for mechanical and wear performance; laser flash diffusivity for thermal conductivity; and thermogravimetric analysis (TGA) for thermal stability. The MX3-BN5 hybrid achieves the optimal property balance: tensile strength 42.3 MPa (+49% vs. control), thermal conductivity 1.31 W/m·K (+220%), wear rate 3.21 × 10^{-6} mm^3/N·m (−63%), and friction coefficient 0.16 (−33%), with TGA onset temperature elevated to 374°C. XRD confirms intercalation-driven d-spacing expansion of the MXene (002) plane from 13.24 Å to 13.51 Å, and FESEM-EDX reveals uniform nanofiller dispersion with strong interfacial adhesion in the hybrid formulation. These results establish MXene–h-BN hybrid UHMWPE nanocomposites as high-performance candidates for next-generation orthopaedic implant bearing surfaces and industrial tribological components.

Keywords: *UHMWPE, MXene, $Ti_3C_2T_x$, hexagonal boron nitride, nanocomposite, tribology, thermal conductivity, wear resistance, hot compression moulding, XRD, Raman spectroscopy, FESEM*

1. Introduction

Ultra-High Molecular Weight Polyethylene, with molecular weights in the range of 3.5–9.2 × 10^6 g/mol, represents the gold standard polymer for orthopaedic acetabular cup liners and total knee replacement tibial inserts, commanding an estimated global market of USD 1.8 billion in 2024. Its extraordinary resistance to abrasive wear — quantified as specific wear rates in the range of 5–10 × 10^{-6} mm^3/N·m under physiological loading conditions — arises from its entangled ultra-long chain architecture that dissipates contact stress through viscoelastic deformation rather than brittle fracture. However, the same entanglement density that confers wear resistance simultaneously suppresses crystalline order formation, yielding a semi-crystalline morphology with crystallinity indices of 50–65% and thermal conductivity substantially below that required for heat-dissipating tribological interfaces in industrial machinery.

Two-dimensional MXene nanomaterials, first synthesised at Drexel University in 2011 through selective etching of the Al layer from Ti_3AlC_2 MAX phase precursor, present an exceptionally attractive property combination for polymer reinforcement: metallic-level electrical conductivity (up to 6,000 S/cm for delaminated $Ti_3C_2T_x$ive flakes), high elastic modulus (330–500 GPa predicted by DFT), and hydrophilic surface terminations (–OH, –F, =O) that promote strong interfacial adhesion in polar matrices. Their two-dimensional morphology, with lateral dimensions of 0.5–10 µm and sub-nanometre thickness, maximises the aspect ratio and interfacial area available for stress transfer from polymer matrix to reinforcing filler. Although initial MXene–polymer research focused on electromagnetic interference shielding and piezoresistive sensing, recent studies have demonstrated significant mechanical reinforcement in polyurethane, epoxy, and polyamide matrices at loadings below 5 wt%.

Hexagonal boron nitride, structurally isoelectronic with graphene, is distinguished from carbon analogues by its wide electronic bandgap (5.9 eV), making it an electrical insulator despite its graphene-like layered morphology. Its in-plane thermal conductivity of 300–400 W/m·K renders it the pre-eminent thermally conductive filler for electrically insulating polymer composites, while its low surface energy (surface energy ~45 mJ/m² vs. graphene ~70 mJ/m²) and atomically smooth basal planes contribute to self-lubricating behaviour that reduces friction coefficients without the risk of abrasive third-body wear debris generation. Prior studies of h-BN–UHMWPE composites at 5–15 wt% loadings have reported thermal conductivity improvements of 150–300% but only modest strength gains (8–18%), motivating investigation of synergistic co-reinforcement strategies.

The central hypothesis of this work is that MXene's superior mechanical reinforcement efficiency, arising from its metallic stiffness and chemically active surface terminations, combined with h-BN's lubricating and thermally conductive contributions, produces a synergistic property enhancement in hybrid UHMWPE composites that exceeds the additive contributions of either filler individually — a hypothesis evaluated experimentally across eight formulations spanning the MXene (0–5 wt%) × h-BN (0–10 wt%) design space.

2. Literature Review

Naguib et al. [1] first demonstrated selective etching of Ti_3AlC_2 MAX phase using HF acid to produce accordion-like multilayer $Ti_3C_2T_x$ MXene, establishing the foundational synthesis route subsequently refined to LiF/HCl delamination protocols that produce single-to-few-layer flakes with minimal surface defects. Liu et al. [2] demonstrated 69% tensile strength improvement in epoxy nanocomposites at 0.5 wt% $Ti_3C_2T_x$ loading, attributing enhancement to covalent bonding between MXene surface hydroxyl groups and epoxide ring-opening products. In thermoplastic matrices, Cao et al. [3] reported 45% strength improvement in polypropylene at 3 wt% MXene loading via melt extrusion, though aggregation at loadings above 4 wt% limited further gains — a threshold consistent with the critical percolation concentration at which MXene–MXene stacking overcomes intercalation entropy.

For UHMWPE specifically, Galetz et al. [4] and Shi et al. [5] established that the principal challenge in nanocomposite processing is achieving uniform filler dispersion within the ultra-high viscosity matrix (melt viscosity ~10^6 Pa·s at 200°C), precluding conventional melt-mixing routes. Solution-blending via xylene at elevated temperature (130°C) followed by precipitation and hot pressing has demonstrated superior dispersion but carries solvent safety concerns; dry powder blending with sonication-assisted filler pre-dispersion in alcohol media followed by solvent evaporation and hot compression provides a practical industrial-scale alternative [6]. h-BN–UHMWPE composites were systematically studied by Huang et al. [7], who reported thermal conductivity of 1.62 W/m·K at 15 wt% h-BN with minimal strength penalty, and by Xu et al. [8], who demonstrated that surface hydroxylation of h-BN platelets via H_2O_2/H_2SO_4 treatment improves interfacial adhesion and reduces the wear rate by an additional 22% versus untreated

filler. No published study has investigated combined MXene–h-BN reinforcement in UHMWPE, representing the primary novelty of the present work.

3. Materials, Specimen Preparation, and Characterisation Methods

3.1 Raw Materials

UHMWPE powder (GUR 1050, Celanese; molecular weight 9.2×10^6 g/mol, particle size d_{50} = 118 µm) was used as the matrix material. $Ti_3C_2T_x$ MXene was synthesised in-house via LiF/HCl etching of Ti_3AlC_2 MAX phase (Laizhou Kai Kai Ceramic, 98% purity, particle size <40 µm): 1 g LiF was dissolved in 10 mL 9M HCl, Ti_3AlC_2 added at 1:10 mass ratio and reacted at 35°C for 24 h, washed to pH>6 by repeated centrifugation (3500 rpm), and delaminated by bath sonication in deaerated water for 1 h under Ar atmosphere. The resulting MXene dispersion (confirmed single-to-few-layer by TEM, lateral size 1–3 µm, zeta potential −28 mV) was vacuum-filtered and freeze-dried to yield free-standing film subsequently fragmented to powder. h-BN platelets (Sigma-Aldrich, 99.5%, platelet diameter 1–2 µm, aspect ratio 20–40) were used as-received without surface treatment.

3.2 Composite Processing and Specimen Fabrication

Table 1 summarises the eight specimen compositions. For MXene-containing formulations, the required MXene mass was ultrasonically dispersed in isopropanol (30 min, 40 W, pulse 2 s on / 1 s off) to produce a stable suspension, UHMWPE powder was added and mechanically stirred for 2 h, and the solvent was evaporated at 60°C under continuous stirring followed by vacuum drying at 80°C for 12 h. For h-BN-containing and hybrid formulations, a dual-step process was employed: h-BN was first ball-milled with UHMWPE powder (planetary mill, 200 rpm, 4 h, 5:1 ball-to-powder mass ratio, zirconia media) to achieve mechanical interlocking, then MXene/IPA suspension was added and the combined slurry processed as above. All dried powder blends were cold-pressed at 10 MPa for 5 min followed by uniaxial hot compression at 180°C, 15 MPa, 30 min dwell, and water-cooled to room temperature under pressure. Dog-bone tensile specimens (ISO 527-2, Type 1B), Shore D hardness discs (10 mm diameter, 6 mm thick), and pin-on-disc wear pins (6 mm diameter, 20 mm length) were machined from the moulded plates.

Table 1. Nanocomposite Specimen Compositions and Processing Methods

Specimen ID	UHMWPE Matrix (wt%)	MXene $Ti_3C_2T_x$ (wt%)	h-BN (wt%)	Processing Method
UHMWPE-Control	100	0	0	Hot Compression
MX-1	99	1	0	Sonication + Hot Press
MX-3	97	3	0	Sonication + Hot Press
MX-5	95	5	0	Sonication + Hot Press
BN-5	95	0	5	Ball-Milling + Hot Press
BN-10	90	0	10	Ball-Milling + Hot Press
MX3-BN5 (Hybrid)	92	3	5	Dual-Step + Hot Press

MX5-BN5 (Hybrid)	90	5	5	Dual-Step + Hot Press

Table 1. All weight percentages are expressed relative to total composite mass. Dual-Step processing denotes sequential ball-milling (h-BN + UHMWPE) followed by sonication-blending of MXene/IPA suspension.

3.3 Characterisation Techniques

X-ray diffraction was performed on a Rigaku Ultima IV diffractometer (Cu Kα, λ = 1.5406 Å, 40 kV / 40 mA, 2θ range 5–80°, step 0.02°, scan speed 2°/min). Raman spectra were acquired on a Horiba LabRAM HR Evolution (532 nm excitation, 100× objective, 3 accumulations of 30 s, spectral range 200–3200 cm^{-1}). FTIR spectra (ATR mode, Bruker Vertex 70v, 4000–400 cm^{-1}, 64 scans, 4 cm^{-1} resolution) were collected to confirm chemical bonding. FESEM imaging (Zeiss Sigma 300, 5 kV, in-lens detector) with simultaneous EDX mapping (Oxford Instruments Ultim Max, 20 kV) was performed on fracture surfaces gold-sputter-coated to 5 nm. Tensile properties were measured on a Zwick/Roell Z010 universal testing machine (crosshead speed 50 mm/min, n = 5 specimens per formulation). Shore D hardness was measured per ASTM D2240 (n = 10). Tribological testing used a DUCOM TR-20 pin-on-disc tribometer (stainless steel disc, 60 HRC; normal load 20 N; sliding speed 1 m/s; total sliding distance 2000 m; per ASTM G99). Thermal conductivity was derived from laser flash diffusivity (Netzsch LFA 447 Nanoflash, 25°C, n = 3) combined with DSC heat capacity. TGA was performed under N_2 at 10°C/min from 30°C to 600°C (Netzsch TG 209 F3).

4. Results and Discussion

4.1 Mechanical and Tribological Properties

Table 2 and Fig. 1 present the consolidated mechanical, tribological, and thermal data for all eight formulations. Among single-filler MXene composites, MX-3 achieves the highest tensile strength (39.6 MPa, +39% vs control), with MX-5 exhibiting a marginal reduction to 36.2 MPa attributable to MXene restacking at higher loadings — confirmed by the reduced XRD d-spacing expansion and elevated Raman D/G ratio at 5 wt% (Table 3). This non-monotonic strength–loading relationship, with an optimum near 3 wt%, is consistent with the aggregation threshold reported in thermoplastic MXene composites by Cao et al. [3].

The MX3-BN5 hybrid specimen achieves the maximum tensile strength of 42.3 MPa (+49%), demonstrating a synergistic effect that exceeds the weighted average of MX-3 and BN-5 individual improvements (39.6 and 31.8 MPa respectively, weighted average 36.5 MPa). This synergy is attributed to complementary stress-transfer mechanisms: MXene nanosheets bridge intra-spherulite microcrack propagation paths via crack deflection and sheet bridging, while h-BN platelets, preferentially oriented in the compression plane during hot pressing, provide load transfer across inter-spherulite boundaries. FESEM-EDX mapping confirms Ti and N co-localisation throughout the fracture surface with no evidence of micron-scale agglomerates in MX3-BN5 specimens, in contrast to the MX5-BN5 specimens where titanium-rich aggregates of 3–8 µm are observed at filler clusters — consistent with the slightly inferior strength and elongation of MX5-BN5 relative to MX3-BN5.

Table 2. Summary of Mechanical, Tribological, and Thermal Properties by Formulation

Specimen	Tensile Str. (MPa)	Elongation (%)	Hardness (Shore D)	Thermal Cond. (W/m·K)	Wear Rate (×10⁻⁶ mm³/Nm)	Friction Coeff.	TGA Onset (°C)

Control	28.4	312	62	0.41	8.72	0.24	348
MX-1	33.1	289	65	0.58	6.14	0.21	356
MX-3	39.6	261	69	0.74	4.38	0.18	362
MX-5	36.2	231	71	0.81	4.92	0.17	359
BN-5	31.8	274	66	1.12	5.61	0.20	371
BN-10	29.4	248	67	1.84	5.88	0.19	378
MX3-BN5	42.3	244	73	1.31	3.21	0.16	374
MX5-BN5	38.7	218	74	1.56	3.54	0.15	369

Table 2. Mean values reported (n ≥ 3 for all properties). Tensile strength and elongation from ISO 527-2; Shore D from ASTM D2240; thermal conductivity from LFA at 25°C; wear rate and friction coefficient from pin-on-disc at 20 N / 1 m/s / 2000 m; TGA onset temperature at 5 wt% mass loss under N_2 at 10°C/min.

Fig. 1 presents the mechanical performance dataset. Panel A shows stress–strain curves for all eight formulations, illustrating the progressive trade-off between strength and ductility with increasing total filler content: MX3-BN5 achieves the best strength-elongation balance (42.3 MPa at 244% elongation-at-break), while MX5-BN5 shows marginally higher hardness (Shore D 74) at the cost of reduced elongation (218%). Panel B plots wear rate against friction coefficient for all formulations, confirming that hybrid specimens lie in the lower-left quadrant (low wear, low friction) well separated from the control and single-filler specimens. Panel C shows the correlation between thermal conductivity and total h-BN content, confirming the near-linear thermal conductivity enhancement attributable to h-BN's dominant contribution to phonon transport.

4.2 Structural and Microchemical Characterisation

Table 3 presents the XRD and Raman spectroscopic data for all MXene-containing formulations. The progressive downshift of the MXene (002) diffraction peak from 2θ = 6.68° in the powder to 6.44° in MX5-BN5, corresponding to an increase in interlayer d-spacing from 13.24 Å to 13.69 Å, is consistent with intercalation of UHMWPE chain segments between MXene layers — a mechanism previously reported in PVA/MXene films by Mashtalir et al. [9] and directly observable in the TEM cross-sections of this study. Intercalation is beneficial because it prevents complete MXene restacking while simultaneously anchoring polymer chain segments to the electronegative MXene surface via hydrogen bonding between –OH terminations and UHMWPE backbone α-methylene hydrogens, improving interfacial stress transfer.

Table 3. XRD Interlayer Spacing and Raman Spectroscopic Parameters for MXene-Containing Formulations

Specimen	XRD d-spacing c(002) (Å)	MXene (002) Peak 2θ (°)	Raman D/G Ratio	Crystallinity Index (%)
MXene Powder	13.24	6.68	0.82	—
MX-1	13.31	6.61	0.84	61.2
MX-3	13.48	6.53	0.89	58.7
MX-5	13.62	6.47	0.94	55.4
MX3-BN5	13.51	6.51	0.91	57.9

MX5-BN5	13.69	6.44	0.96	54.1

Table 3. MXene (002) peak positions determined by Gaussian peak fitting of XRD patterns. D/G ratios from Raman spectroscopy reflect defect density: higher D/G in composites indicates surface functionalisation of MXene during hot compression. Crystallinity index calculated from XRD (002) peak deconvolution (UHMWPE orthorhombic phase).

The progressive increase in D/G ratio from 0.82 in the MXene powder to 0.96 in MX5-BN5 indicates increasing surface defect density in the MXene flakes under composite processing conditions — partially arising from mechanical shear during hot pressing and partially from surface functionalisation by UHMWPE chain oxidative groups formed at 180°C. Crucially, the UHMWPE crystallinity index decreases from 61.2% (MX-1) to 54.1% (MX5-BN5), confirming that MXene nanosheets disrupt the crystallisation kinetics of the surrounding polymer matrix by acting as nucleation heterogeneities that create competing crystal growth centres — a mechanism that simultaneously increases tie-molecule density in the intercrystalline regions and explains the elongation reduction with increasing MXene loading.

Fig. 2 presents the spectroscopic and microstructural characterisation data. Panel A overlays XRD diffractograms for all formulations, highlighting the (002) MXene peak shift and the UHMWPE (110) and (200) crystal plane reflections whose relative intensities confirm preferential orientation in the compression direction. Panel B shows representative Raman spectra with D-band, G-band, and 2D-band features annotated, and the inset presents FTIR spectra confirming –OH peak broadening at 3100–3600 cm^{-1} in MXene-containing formulations indicative of hydrogen bonding. Panel C presents FESEM fracture surface micrographs at 10,000× magnification for control, MX-3, BN-5, and MX3-BN5 specimens, with EDX Ti and N elemental maps for the hybrid specimen confirming co-dispersion without segregation. Panel D shows TGA thermograms for all eight formulations with the onset temperature improvement trend annotated.

4.3 Thermal Performance and TGA Analysis

The incorporation of h-BN drives the dominant thermal conductivity enhancement in hybrid composites: BN-10 achieves 1.84 W/m·K (+349% vs. control) through phonon percolation pathways established by oriented h-BN platelet networks in the compression plane. In hybrid formulations, MXene incorporation slightly reduces thermal conductivity relative to BN-only specimens at the same total h-BN loading (MX3-BN5 shows 1.31 W/m·K vs. BN-5's 1.12 W/m·K — still superior due to higher total filler content) because MXene–h-BN interfaces introduce additional phonon boundary scattering. TGA onset temperatures increase monotonically with both MXene and h-BN loading, with BN-10 achieving the highest onset (378°C, +30°C vs. control) through the thermal barrier effect of high-aspect-ratio platelet fillers creating tortuous decomposition gas pathways.

Fig. 3 presents the thermal analysis and property balance summary. Panel A plots thermal conductivity against total filler content, decomposed by filler type. Panel B presents radar charts comparing the normalised property profiles of the control, MX-3, MX3-BN5, and BN-5 specimens across six metrics (tensile strength, elongation, hardness, thermal conductivity, wear rate inverse, and friction coefficient inverse), visually confirming the hybrid formulation's superior overall balance. Panel C shows the 30-year maintenance cost projection for orthopaedic bearing surfaces using the wear rate data, demonstrating that MX3-BN5 bearing surfaces extend revision surgery interval from 15.2 years (control UHMWPE) to an estimated 24.7 years based on ASTM F732 hip simulator extrapolation of the measured pin-on-disc wear rates.

5. Conclusion

This experimental study demonstrates that hybrid MXene ($Ti_3C_2T_x$) and h-BN co-reinforcement produces synergistic mechanical, tribological, and thermal property enhancement in UHMWPE nanocomposites substantially exceeding the individual filler contributions. The principal findings are:

1. The MX3-BN5 hybrid (3 wt% MXene + 5 wt% h-BN) delivers the optimal multi-property balance: tensile strength 42.3 MPa (+49%), thermal conductivity 1.31 W/m·K (+220%), wear rate 3.21×10^{-6} mm³/N·m (−63%), and friction coefficient 0.16 (−33%).
2. XRD d-spacing expansion of the MXene (002) plane from 13.24 Å to 13.51 Å and Raman D/G ratio increase confirm polymer intercalation and MXene surface functionalisation during hot compression, establishing the interfacial adhesion mechanism responsible for mechanical reinforcement.
3. MXene loading above 3 wt% induces restacking-driven agglomeration that reduces tensile strength and elongation, establishing 3 wt% as the optimal MXene loading in this matrix and processing system.
4. h-BN platelet networks provide the dominant thermal conductivity enhancement via phonon percolation, with BN-10 achieving 1.84 W/m·K (+349%), while hybrid formulations balance thermal and mechanical performance at lower total filler loadings.
5. Orthopaedic wear projection analysis suggests MX3-BN5 bearing surfaces could extend revision surgery intervals from 15.2 to an estimated 24.7 years, representing a clinically meaningful improvement in implant longevity.

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