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Evidence on the Electronic structure of UHMWPE/Mxene Nanocomposites Using Advanced X-Ray Absorption Technique

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Introduction: A vast family of transition metal carbides, nitrides, or carbonitrides with a wide range of aspect ratios and thin atomic layer thickness known as MXenes. Mxenes are electrically conductive, hydrophilic, layered, two-dimensional (2D) nanomaterials. A single-layer MXene is optically transparent which approximately absorbs 3% of visible light. The general formula of MXenes is $M_{n+1}X_nT_x$, where M signifies an early transition metal such as Ti, X is carbon and/or nitrogen, T is a surface functional group such as OH, F, and O, and x is the number of functional groups. The value of n is an integer between 1 to 3. The most-studied MXene is Ti_3C_2 **[1]**.

By combining MXenes (Ti_3C_2) with polymers to create Ti_3C_2/polymer composites, it is possible to improve the tribological and mechanical properties of polymers. Despite having limited mechanical qualities, ultra-high molecular weight polyethylene (UHMWPE) is chemically inert, lubricious, and resistant. As a result of the combination of $Ti_3C_2T_x$ with Ultra-High Molecular Weight Polyethylene (UHMWPE), a thermoplastic polyethylene composite with a long chain character is created, which can then be changed into a strong thermoplastic by applying pressure and heat. UHMWPE was more practical due to its anti-corrosive, low-abrasive, and moisture-resistant properties. Their mechanical qualities are improved by the higher Ti_3C_2 concentrations. The crystallinity rises as the coefficient of friction falls simultaneously. Additionally, it functions as a lubricant similar to graphene. The composite, therefore, has better characteristics than pure MXene. They can reject moisture for conveyor belts, marine equipment, food processing, etc. due to their decreased moisture absorption capacity. In a similar way, the electronic and magnetic characteristics of the material can also be varied in order to have its application in energy storage devices and shall also pave the way for many other practical implications **[2-3]**.

In the current study, we report the study on the Synthesis and electronic spectra of hot-press synthesized nanocomposites. As, the electronic characteristics of this complex system, remain poorly known despite significant research efforts. We used a sophisticated analytical synchrotron-based approach in this research to disclose the electronic structures of UHMWPE/Mxene (0.5wt%) nanocomposites.

Experiment: The processing of UHMWPE/MXene nanocomposites were prepared by solution process followed by compression molding technique. These composites were prepared in two consecutive steps. Initially, the solution dispersion process was used to prepare UHMWPE/MXene mixed powders with different loading concentrations of MXene (0.5 wt. %.). Ti_3C_2 (MXenes) were added to ethanol and then intense dispersion was achieved by ultra-sonicated for 1 hour. In the meanwhile, UHMWPE powder was poured into ethanol and followed by high-speed stirring for two hours at temperature 110 °C. The stable MXene/ethanol solution was then quickly dropped into the ethanol/UHMWPE solution and the final solution was stirring at the speed of 400 rpm and temperature about 110 °C to completely evaporate the ethanol solvent. During the stirring process, polymer granules swell and MXenes and magnetic particles were decorated on the surface of the neat polymer. Finally, UHMWPE/MXene powders were compression molded with a hot press for 15 min, at 150 °C to form a rectangular strip of approximately 3mm thickness, 50mm length and breadth 50 mm.

Results and Discussions: The sample's purity was checked using a non-destructive X-ray powder Diffraction approach, which showed no sign of contamination. Studies on X-ray spectroscopy, scattering, and imaging were carried out at the variable polarisation soft x-ray beam-line BL-16A of the Photon Factory (KEK, Japan). The experimental geometry for soft X-ray absorption (XAS) studies is shown in Figure 1. The sample was placed with a 5 T superconducting magnet in the 10^{-9} Torr vacuum chamber. Near the Ti $L_{2,3}$ absorption edges, XAS signals were detected with an energy resolution of 0.1 eV utilizing the surface-sensitive total electron yield (TEY) mode **[4-7]**.

The Ti *L*edge XAS spectra of a UHMWPE/Ti_3C_2 nanocomposite are shown in Figure 1. The XAS spectrum of Ti at $L_{3,2}$-edge revealed a more complicated structure as a result of the consequences of atomic interactions and crystal field effects. Furthermore, as seen in Figure, the crystal field causes the splitting of the L_3 and L_2 edges into $t_{2\,g}$ (L_2 and L_3) and *eg* (L_2 and L_3) levels. The primary reason for studying the Ti L_3 edge was to investigate the influence of UHMWPE mixing into the Ti_3C_2 system. The L_3 ($2p_{3/2}$→3d) (456-462 eV) and L_2 ($2p_{1/2}$→3d) (462-469 eV) transitions each contribute to the Ti *L*-edge XAS. Ti *L*-edge XAS spectra are in good agreement with the findings of Zhang *et al*. **[8]**. The spectral characteristics of the Ti $L_{3,2}$ edge of UHMWPE/ Ti_3C_2 nanocomposites were compared to TiO_2 spectra, the spectral structures resemble TiO_2 spectra. Furthermore, the spin-orbit splitting value of the TCO sample at Ti $L_{3,2}$ edges has been experimentally measured to be ~5 eV. This value is found similar to the spin-orbit splitting value for rutile and anatase TiO_2.

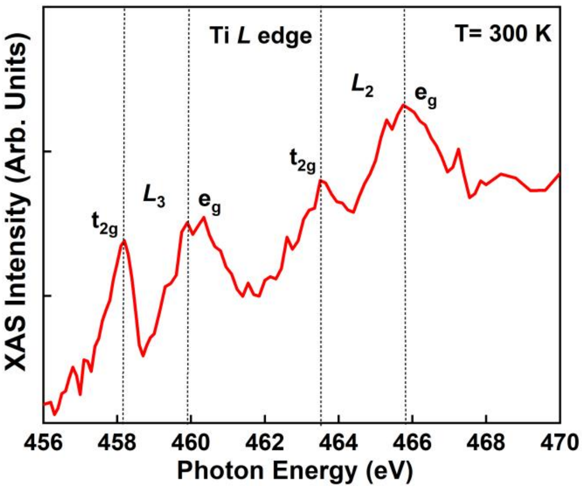

Figure 1. Normalized XAS spectra at Ti $L_{2,3}$-edge.

As a result of the comparison, it is possible to infer from XAS spectra that the Ti_3C_2 component of the complex nanocomposite of UHMWPE/Ti_3C_2 contains titanium in the +4 oxidation state. As, the mixture of polymer and Mxene nanocomposites donot show any magnetization behaviour which was evident from the X-ray magnetic circular di-chroism **[4]** study. Therefore, we can draw a conclusion from the current study that the addition of any spinel oxides into this complex system will ultimately result in the origin of magnetization in this mutifunctional system. Our future work, shall be dedicated to introduce $NiFe_2O_4$ into the UHMWPE/Ti_3C_2 nanocomposite, with varying contents of Mxene. We shall note down the impact of Mxene contents and $NiFe_2O_4$ on the magnetization behaviour of the material.

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