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Electronic and Magnetic characterization of 2-dimensional UHMWPE/Mxene/$NiFe_2O_4$ Nano-composites Using Advanced X-Ray Magnetic Circular Dichroism study

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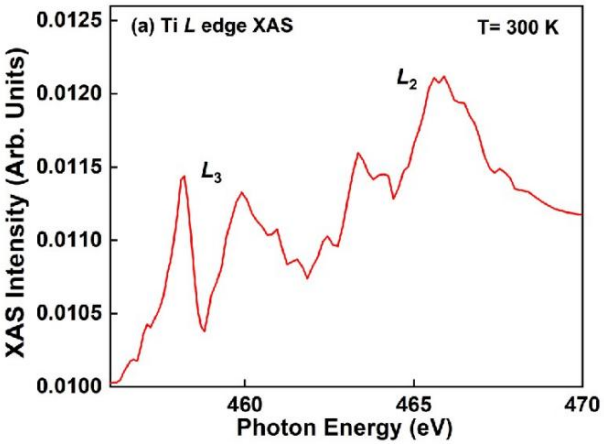
Introduction: MXenes are a brand-new class of 2-dimensional materials that are produced by selective etching of the A layers off the $M_{n+1}AX_n$ (MAX) phases. MAX phases are ternary carbides or nitrides with the general formula $M_{n+1}AX_n$, where M is a transition metal, A is an A-group element (often group IIIA or IVA), X is either C or N or CN, and the value of n can be 1, 2, or 3. A variety of MAX phases can be used to modify the composition of MXenes, which have a lamellar structure similar to that of graphene. MXenes are a novel class of 2-D materials with extraordinary electrical, optical, magnetic and thermoelectric properties similar to graphene that has recently attracted a lot of interest from researchers **[1]**.

MXenes are a very promising additive for improving the tribological and mechanical properties of polymers due to their distinctive electrical properties, excellent mechanical strength and high specific surface area, etc. Although Ti_3C_2 has been studied for usage in several fields as a conventional MXene material, Ti_3C_2/polymer composites have been less explored. Thus, the study of Ti_3C_2/polymer composites has significant practical implications. The excellent characteristics of ultra-high molecular weight polyethylene (UHMWPE), a high-performance engineering thermoplastic, include good biocompatibility, high ultimate tensile strength, self-lubrication, chemical inertness, and the highest wear resistance of all thermoplastics. These qualities make UHMWPE useful in a variety of fields. UHMWPE's applicability is however limited by a few mechanical characteristics **[2]**, including hardness, fatigue strength, and creep resistance. In order to increase its utility, these qualities must be increased. An efficient way to enhance a polymer's mechanical characteristics is by adding inorganic fillers to the polymer. Nanomaterials are a new form of filler that is ideal for polymer matrix composites because of their special characteristics and nanostructures. As fillers for UHMWPE, nanomaterials such as graphene, carbon nanotubes, and ZnO have been thoroughly investigated. The findings demonstrate that nanoscale effects allow the incorporation of nanomaterials to significantly enhance its thermal, tribological and mechanical, properties. However, the past studies does not examine the electronic and magnetic properties of these complicated systems based on UHMWPE/Mxene/$NiFe_2O_4$. The research on these properties is crucial to making this material more and more appropriate for multifunctional systems and has thus far shall help us to identify the most qualified candidates among the 2D-materials that are now available.

In the present work, we report on the study of synthesis and characterization of electronic and magnetic properties of UHMWPE/Mxene (0.5wt%) nano composites. The advanced synchrotron-based X-ray Absorption Spectroscopy (XAS) and X-ray Magnetic Circular Dichroism (XMCD) measurements for the nanocomposite sample was carried out to unveil the magnetization behaviour of the material.

Experiment: A solution procedure and compression molding technique were used to synthesize the UHMWPE/Mxene/

$NiFe_2O_4$ nanocomposites. In two sequential processes, these composites were prepared. UHMWPE/Mxene/ $NiFe_2O_4$ mixed powders were first made using the solution dispersion procedure with 0.5wt% of Mxene loading concentrations in it. After adding Ti_3C_2 (Mxenes) to the ethanol, strong dispersion was accomplished using ultrasonication for one hour. In the meantime, ethanol was added to the UHMWPE powder, which was then stirred vigorously for two hours at a temperature of around 110 °C. The stable Mxene/ $NiFe_2O_4$/ethanol solution was then promptly poured into the ethanol/UHMWPE solution.



F*igure 1(a) Normalised XAS spectra at Ti L edge.*

The combined solution was then stirred at a speed of 400 rpm and a temperature of roughly 110 °C to completely evaporate the ethanol solvent. Granules of the clean polymer swelled as a result of the stirring procedure, and its surface was embellished with Mxenes and magnetic particles. In order to create a rectangular strip with a thickness of roughly 3 mm, UHMWPE/Mxene/$NiFe_2O_4$ powders were compression molded in a hot press for 15 minutes at 150 °C.

By analysing the samples with a Rigaku Smart Lab powder X-ray diffractometer, the substance's purity was confirmed which assured the absence of contaminants in it. Studies on X-ray spectroscopy, scattering, and imaging were carried out using the Photon Factory's variable polarisation soft x-ray beam-line BL-16A at KEK, Japan. Figures 1 depict the experimental geometry for the studies of soft X-ray absorption (XAS) at Ti *L*-edge, where as Figure 2 and 3 represents the XAS and X-ray magnetic circular dichroism (XMCD) spectra at Ni and Fe *L* edge. The sample was placed in the ultra high vacuum chamber of 10^{-9} Torr with the aid of a 5 T superconducting magnet. Using the surface-sensitive total electron yield (TEY) technique close to the Ni $L_{2,3}$ and Fe $L_{2,3}$ absorption edges, the XMCD data was collected. The right and left circularly polarised (RCP and LCP) X-rays were used to measure the XAS and XMCD signals at varying magnetic fields of 0.1T, 1T, and 2T (only the XAS data of 2T has been shown here).

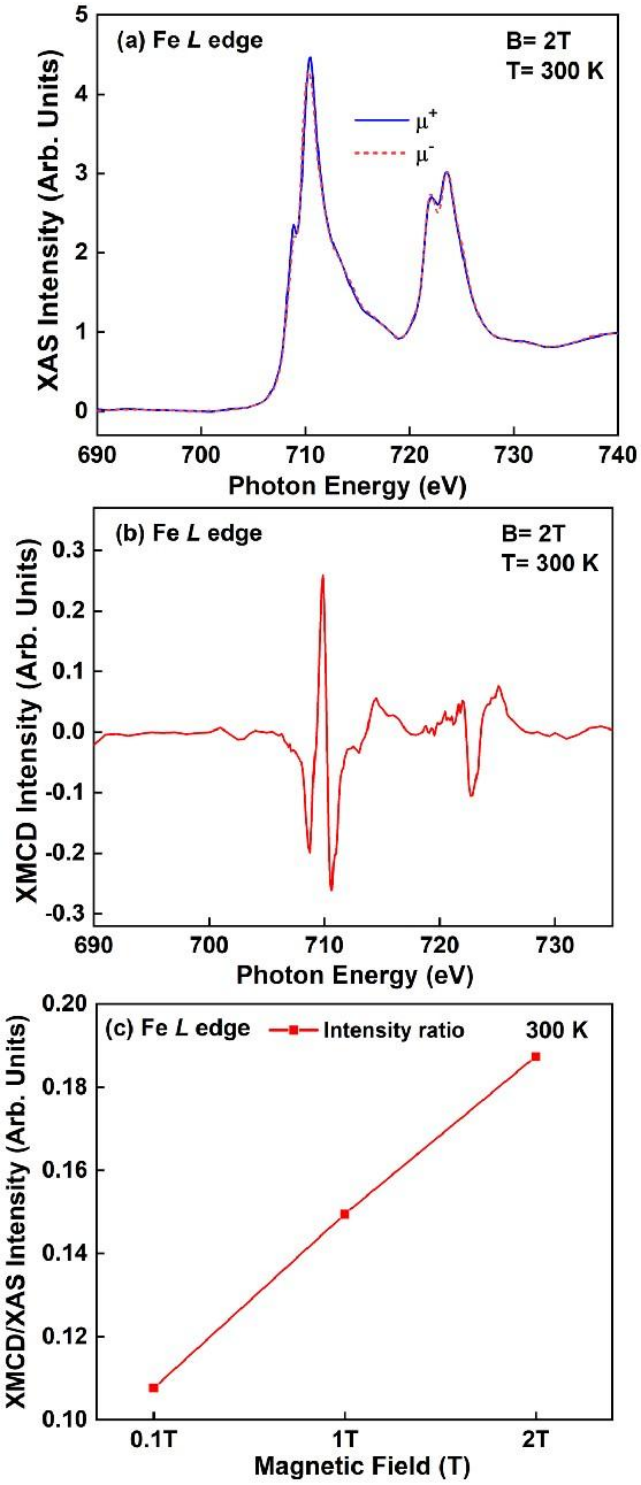


Figure 2(a) Normalised XAS spectra, 2(b) Normalised XMCD spectra of Fe L-edge at applied field of 2T and 2(c) XMCD intensity ratio for Fe L-edge w.r.t applied field of 0.1T, 1T and 2T respectively.

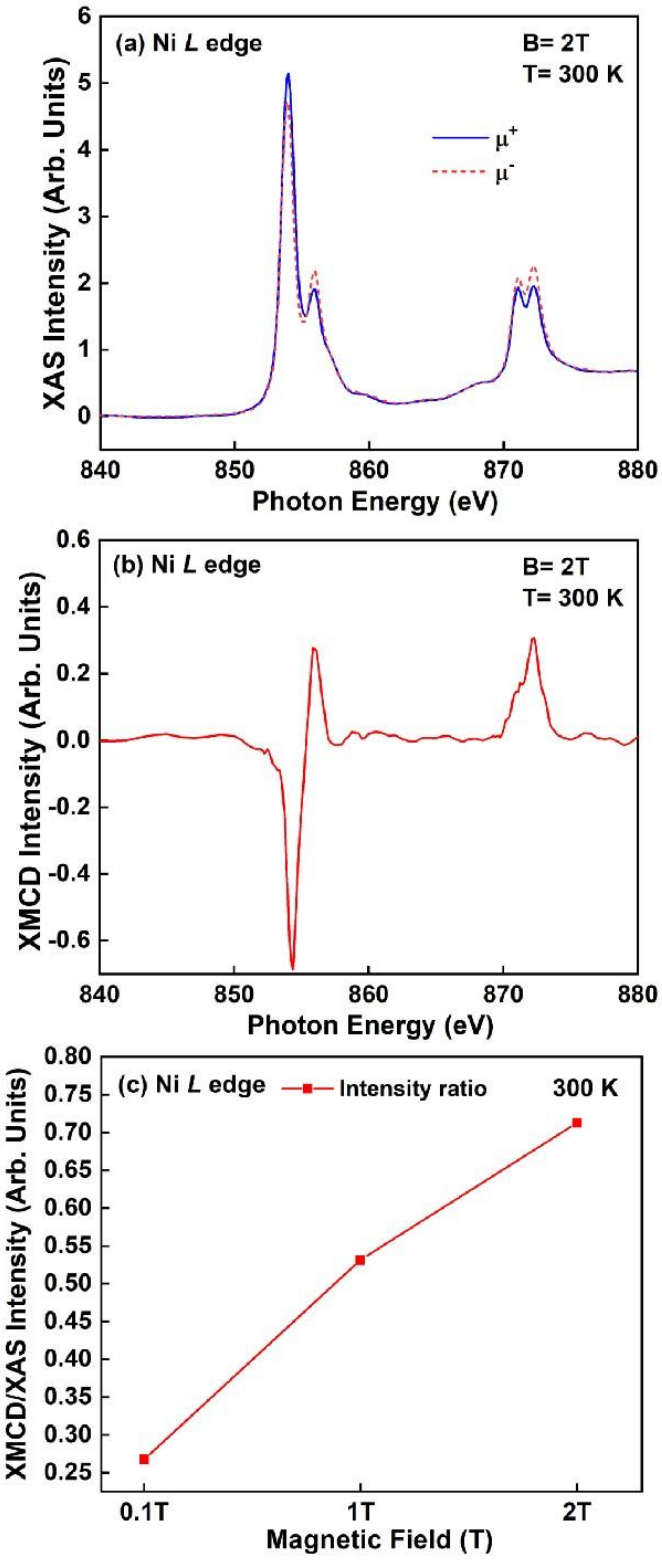


Figure 3(a) Normalised XAS spectra, 3(b) Normalised XMCD spectra of Ni L-edge at applied field of 2T and 3(c) XMCD intensity ratio for Ni L-edge w.r.t applied field of 0.1T, 1T and 2T respectively.

Results and Discussions: Figure. 1. shows the Ti *L*edge XAS spectra of complex nanocomposite. The Ti *L*-edge XAS consists of contributions from L_3 ($2p_{3/2}\rightarrow 3d$) (456–462.8 eV) and L_2 ($2p_{1/2}\rightarrow 3d$) (462–469 eV) transitions. Ti *L*-edge XAS spectra matches well with the zhang *et al* **[3]** findings. Thus based on comparison made, we can conclude that Ti_3C_2 component contains titanium in the +4 oxidation state as far being reported here for complex nanocomposite material of UHMWPE/Ti_3C_2/$NiFe_2O_4$. The XAS spectra that were produced with applied magnetic fields of +2.0 and -2.0T are symbolized by μ^+ and μ^-. Figures 2(a) and 3(a) show left and right circularly polarized light, respectively, which are represented by the symbols μ^+ and μ^- **[4-8]**. By comparing two XAS spectra with negative and positive helicity of the circularly polarized light, the XMCD spectrum was obtained. The experimentally computed XAS spectra for Ni indicated the occupation of divalent Ni at the octahedral sites, whereas the spectrum for Fe aligns well with the trivalent state of Fe at tetrahedral site, and are found to be consistent with Kumari *et al* **[9]**. Qiu *et al* suggested that in the case of Mxene/$NiFe_2O_4$ composite, the increment in the Mxene content led to the enhancement in the grain refinement level which thereby reduced the tendency of Ms but the coercivity rise was clearly noticeable which indicated the transformation of composite from paramagnetic to the ferromagnetic state. The increment in coercivity value in that case, showed the enhanced anisotropic behaviour of nanocomposite material **[10]**.

Although the study on the magnetization behaviour of UHMWPE/Mxene nanocomposite is very scarce and has not been explored yet. The current study suggests that, after addition of $NiFe_2O_4$ into the UHMWPE/Mxene nanocomposite, the magnetization behavior has been significant which is quite visible from the Fe and Ni *L* edge XMCD spectra. Eventually on comparison of the current findings with the sole $NiFe_2O_4$ magnetization result as reported by Klewe *et al* at Ni and Fe edge, it is very clear that the magnetic moment has reduced considerably. The Fe and Ni absorption spectra in the nanocomposite of UHMWPE/Mxene/$NiFe_2O_4$ both exhibit multiplet structures near the *L* edges. It is evident from the Ni *L* edge XAS spectra that Ni has multiple absorption peaks at the L_3 edge, which is located at E= 853.9 and 855.9 eV; in this instance, the L_2 peak exhibits a multiplet feature at 871.04 and 872.26 eV. A doublet structure can be seen in the well-resolved peaks at the Fe L_3 edge's absorption maxima at E = 710.4 eV and 708.8 eV, whilst the L_2 edge's maxima at E = 721.9 and 723.5 eV are clearly discernible. This demonstrates that the localization of Fe 3*d* electrons rather than surface oxidation should be the cause of the fine structures of the Fe $2p \rightarrow 3d$ transition.

Figure 3(b) show XMCD signals obtained for the Ni $L_{2,3}$ edge at the B=2T. Because the t_{2g} level is entirely occupied, the XMCD signal at the Ni L_2 edge is noticeably suppressed, showing magnetic ordering. Figure 1(c) displays the XMCD intensity with respect to the fluctuating magnetic field at 0.1T, 1T, and 2T for Ni and Fe-edges. This outcome is very comparable to the XMCD plots. Figures 2(c) and 3(c) show that the intensity ratio of XMCD decreases as the magnetic field decreases. The magnetization is approaching towards zero with the decrease in the magnitude of the applied field, hence showing the paramagnetic nature of the material. The detailed study of the ongoing work shall be discussed in our future work.

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