Structural and Optical Characterization of titanium-carbide and polymethyl methacrylate based nanocomposite

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ABSTRACT

The rich chemistries and unique morphologies of titanium carbide MXenes made them strong candidates for many applications like sensors and electronic device materials [1]. They can potentially be used as additives to polymers to fabricate composites with outstanding mechanical properties and good electrical conductivities. Presence of titanium-dioxide as a residue of MXene chemical synthesis is researched for it potential benefit on electrochemical properties [2].

In this study we present structural and optical characterization of such polymer nanocomposite titanium-carbide/PMMA (Polymethyl methacrylate) consisting of Ti_3C_2, TiC2 MXenes and TiC, and TiO_2 residues of synthesis in PMMA matrix, as a multicomponent nanocomposite.

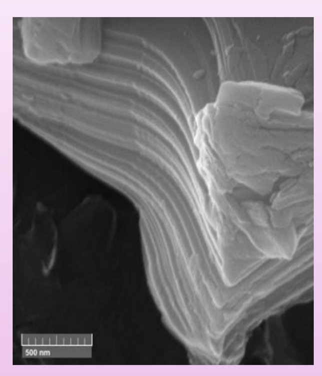
Using XRD, SEM, infrared and Raman spectroscopy, followed by comparative study on the vibrational properties using density functional theory calculations we characterize this nanocomposite.

CALCULATIONS

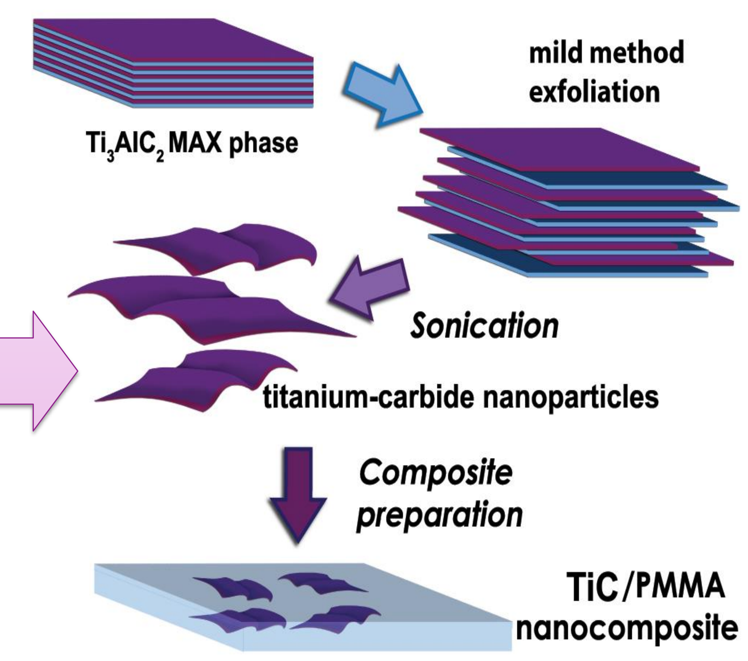
	Titanium-carbide flakes		*PMMA/TiC*		*Description*
	Raman	IR	Raman	IR	
ω1		62.4		66	*Eu, Ti_3C_2*
ω2		85.8		81	*B1, TiO2 rutile*
ω3		119		127	*A_2u, Ti_3C_2 and B_1 TiC_2*
ω4	153				*Eg, Ti_3C_2*
ω5	204	200	204	195	*E, TiO_2 anatase*
ω6	396				*A_2, TiC_2; E, TiO_2 anatase*
ω7	514				*A_1, TiO_2 anatase*
ω8		620		615	*Eu, Ti_3C_2*
ω9	627				*Eg, Ti_3C_2*
ω10			786		*Ag, TiO_2 rutile*
ωP		80		150	
f		1		0.25	

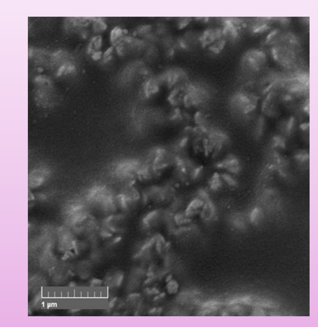
MXene are synthesized by exfoliating MAX phase ternary carbides, nitrides, or carbonitrides: $M_{n+1}AX_n$, where M is an early transition metal, A is a III or IV A-group element and X is carbon/nitrogen. During the synthesis of titanium-carbide MXenes by chemical etching, oxidation can occur which results in presence of TiO_2 consisted of nanosheets and numerous TiO_2 nanocrystals. There are several studies [2,3] whose researched is focused in possible applications of TiO_2-MXene structures. It is demonstrated the synergetic effects of Ti_3C_2 and TiO_2 endowed TiO_2-Ti_3C_2 nanocomposites with excellent properties and improved functionalities. Ti_3C_2 and TiO_2 nanoparticles offered excellent connection between them and facilitated electron exchange. The incorporation of TiO_2 nanoparticles into Ti_3C_2 layers could significantly enhance the electrochemical performance

SYNTHESIS AND STRUCTURAL ANALYSIS

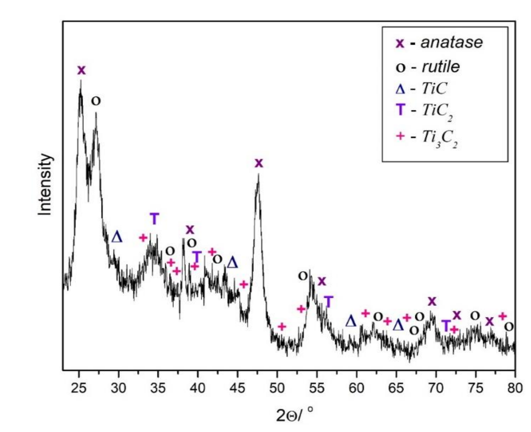


FESEM photo of titanium-carbide flakes delaminated in water



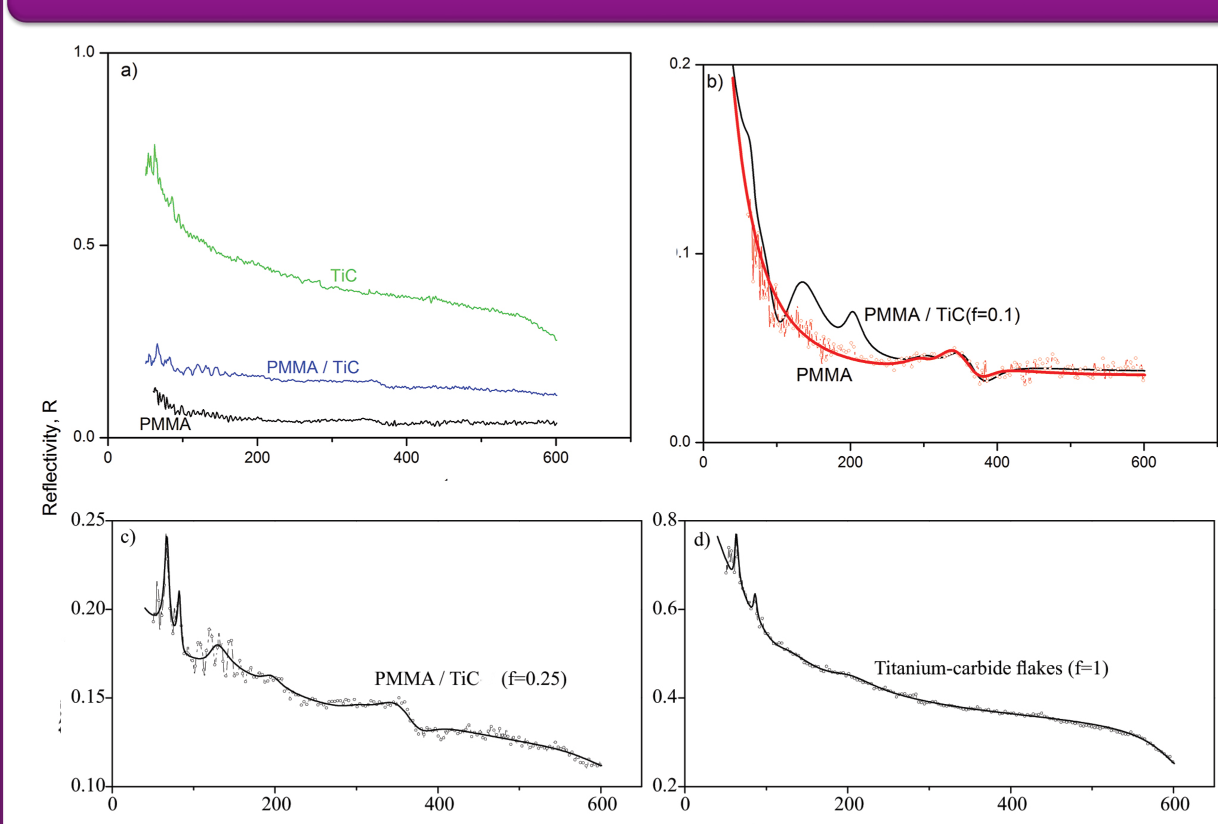


FESEM photo of PMMA nanocomposite prepared with titanium-carbide flakes



XRD pattern for titanium-carbide flakes, starting material for PMMA/TiC nanocomposite

IR SPECTROSCOPY

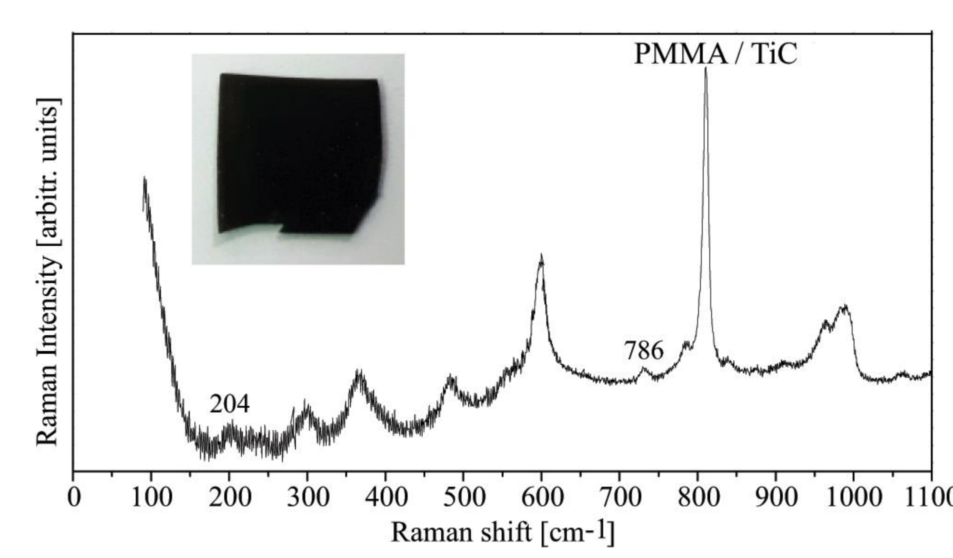


To demonstrate the model, together with the FIR spectrum of PMMA, Figure b is given the theoretical spectrum of PMMA / TiC nanocomposites for f=0.1. The properties of TiC structures are clearly seen. A larger share of TiC structures leads to the spectrum in Figure c, which was obtained for f = 0.25. In Figure d is for f = 1, only pure PMMA.

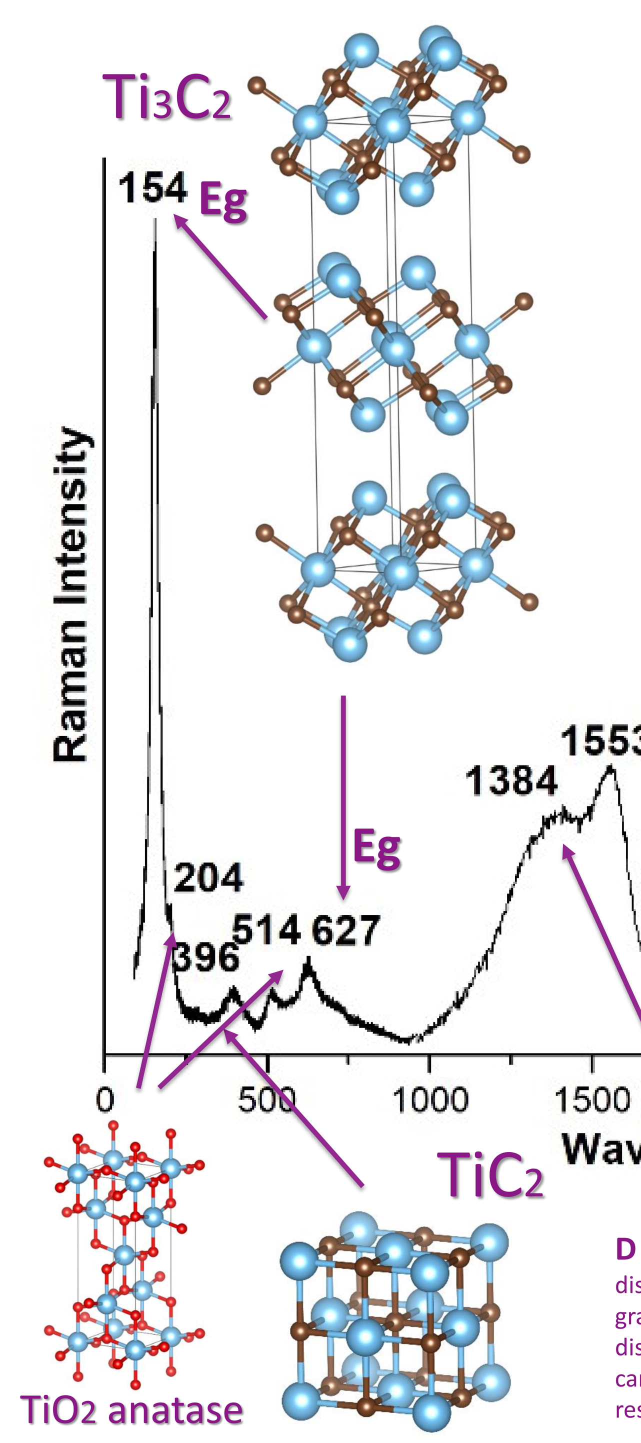
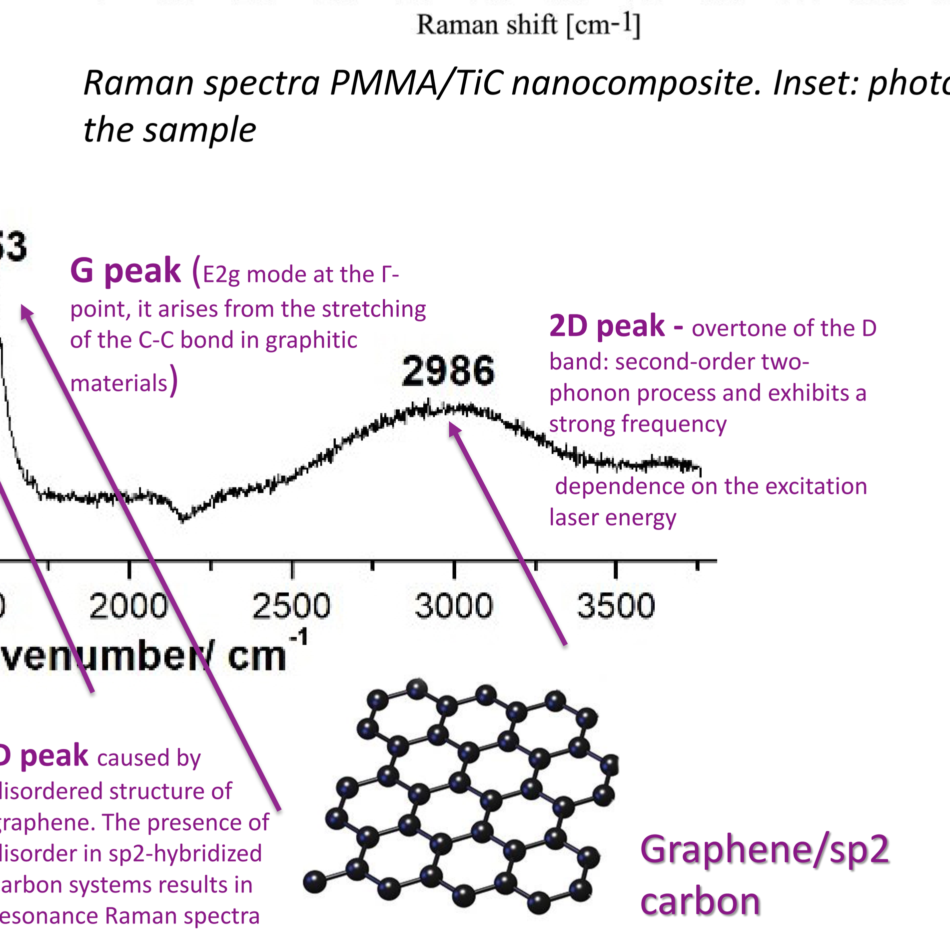
Infrared analysis: a) Infrared spectra of Titanium-carbide flakes (green) and nanocomposites PMMA/TiC (blue) and pure PMMA (black), b) c) and d) circles represent experimental data and solid lines are fit obtained by **Maxwell-Garnet model [5]**

RAMAN SPECTROSCOPY & CALCULATIONS

Raman spectra of TiC flakes before nanocomposite synthesis and assignation of the modes



Raman spectra PMMA/TiC nanocomposite. Inset: photo of the sample

Calculation details

DFT calculations were performed using the **Quantum Espresso software package [4],** based on the plane waves and pseudopotentials. The PBE (Perdew, Burke and Ernzehof) exchange-correlation functional was employed and PAW (Projector augmented waves) pseudopotentials were used. Energy cutoff for wavefunctions and charge density were set to 52 Ry and 575 Ry to ensure the convergence.

Experimental details

MAX PHASE:
M. Barsoum - Department of Materials Science and Engineering, Drexel University, Philadelphia, USA
SAMPLES SYNTHESIS:
I. Pesic - Faculty of Technology and Metallurgy, Belgrade, Serbia
RAMAN SPECTROSCOPY:
M. Gilic – Institute of Physics Belgrade
INFRARED SPECTROSCOPY:
N. Paunovic and N. Romcevic – Institute of Physics Belgrade
XRD:
J. Mitric- Institute of Physics Belgrade
CALCULATIONS
J. Pesic and A. Solajic – Institute of Physics Belgrade

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