Supporting Information

for

Ion Implantation as an Approach for Structural Modifications and Functionalization of $Ti_3C_2T_x$ MXenes

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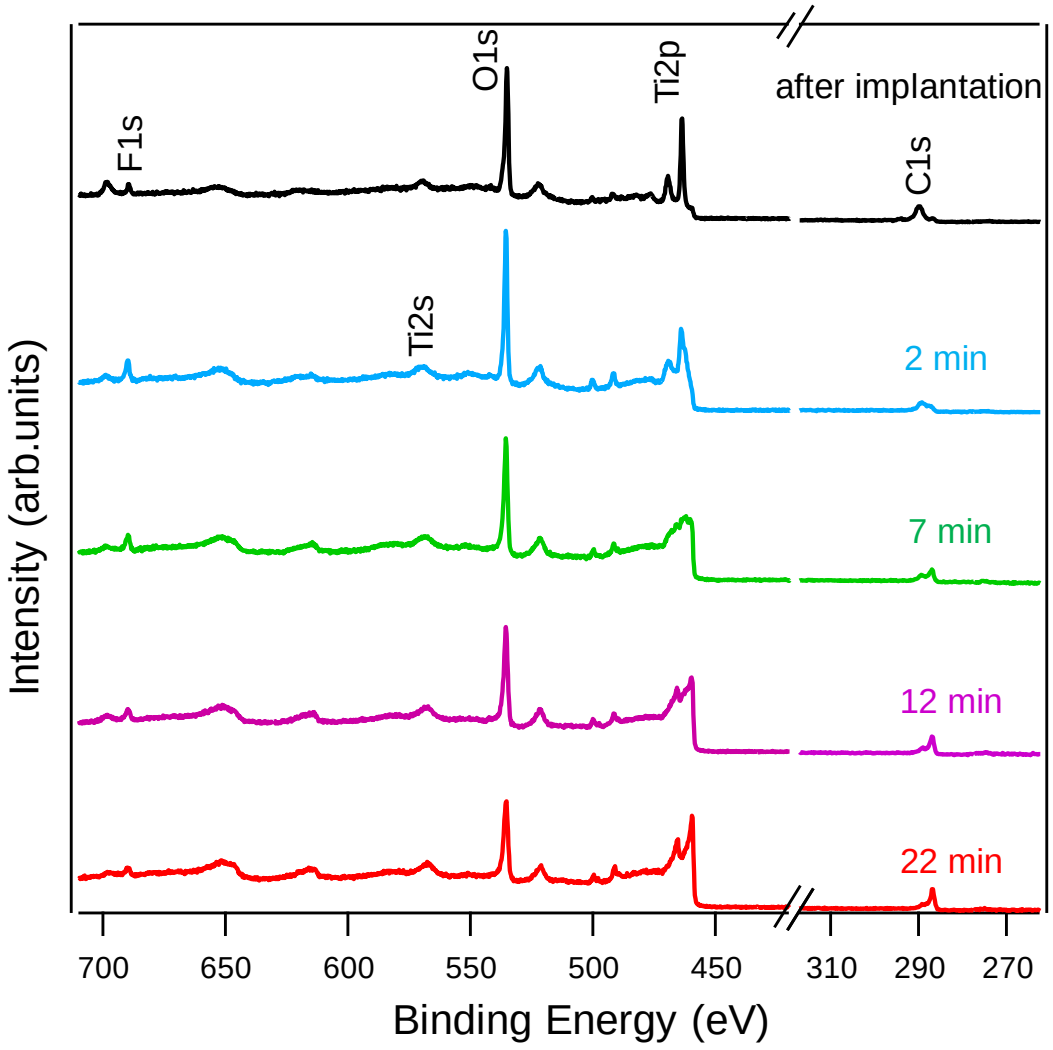


Figure S1. The survey XPS spectra taken on a spin-coated $Ti_3C_2T_x$ film after implantation with $1 \cdot 10^{15}$ Mn-ions/cm^2 at 60 keV and after different 0.5 keV Ar^+ sputtering cycles carried out to remove each time the exposed film surface and have access to the underneath layer.

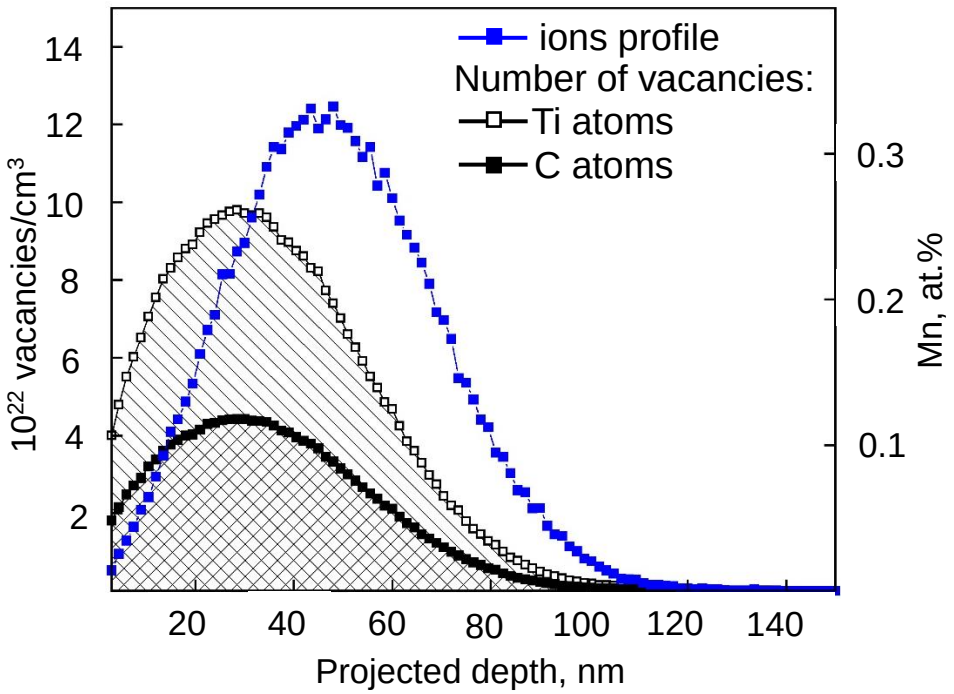
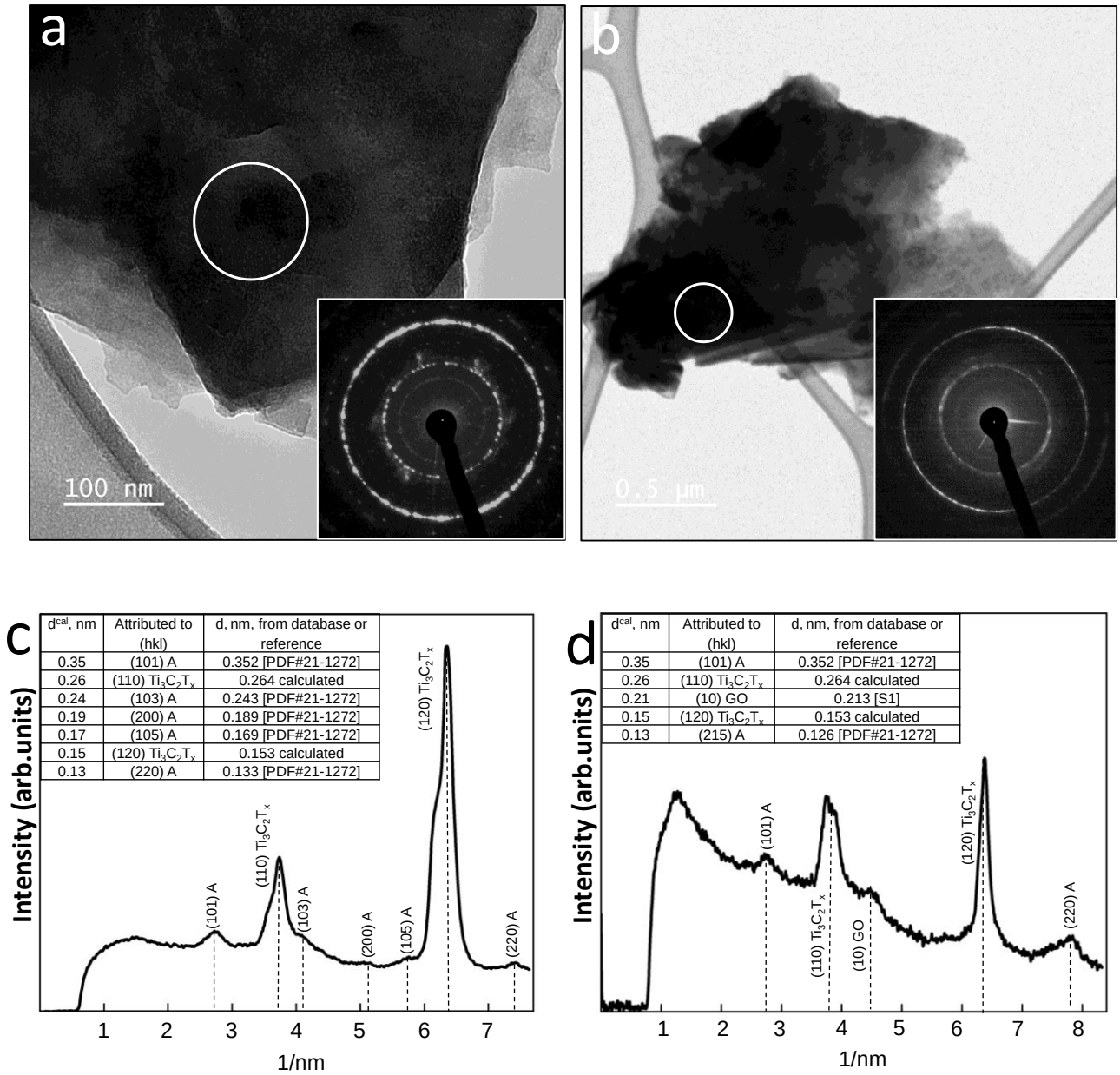


Figure S2. The SRIM simulated depth profiles of Ti and C vacancies (black curves) and Mn^+-ions distribution (blue curve) within the $Ti_3C_2T_x$ thin film following the ion-implantation with $1 \cdot 10^{15}$ ions/cm^2 fluence at 60 keV energy, showing the maximum Mn concentration of ~0.32 at.%.



d^{cal}, nm	Attributed to (hkl)	d, nm, from database or reference
0.35	(101) A	0.352 [PDF#21-1272]
0.26	(110) $Ti_3C_2T_x$	0.264 calculated
0.24	(103) A	0.243 [PDF#21-1272]
0.19	(200) A	0.189 [PDF#21-1272]
0.17	(105) A	0.169 [PDF#21-1272]
0.15	(120) $Ti_3C_2T_x$	0.153 calculated
0.13	(220) A	0.133 [PDF#21-1272]

d^{cal}, nm	Attributed to (hkl)	d, nm, from database or reference
0.35	(101) A	0.352 [PDF#21-1272]
0.26	(110) $Ti_3C_2T_x$	0.264 calculated
0.21	(10) GO	0.213 [S1]
0.15	(120) $Ti_3C_2T_x$	0.153 calculated
0.13	(215) A	0.126 [PDF#21-1272]

Figure S3. The TEM micrograph of thick parts extracted from the spin-coated $Ti_3C_2T_x$ films implanted at $1 \cdot 10^{15}$ (a) and $1 \cdot 10^{16}$ ions/cm² (b) at 60 keV and corresponding energy-filtered (10 eV slit) SAED patterns (insets). (c), (d) The radial intensity profiles of the SAED patterns presented in insets in (a) and (b). d-spacing values, d^{cal}, are calculated from experimental SAED patterns (a, b, insets). Reference values of d-spacings for anatase (A) were taken from JCPDS database – PDF#21-1272. Reference values of d-spacings for graphene oxide (GO) were taken from the Reference S1.

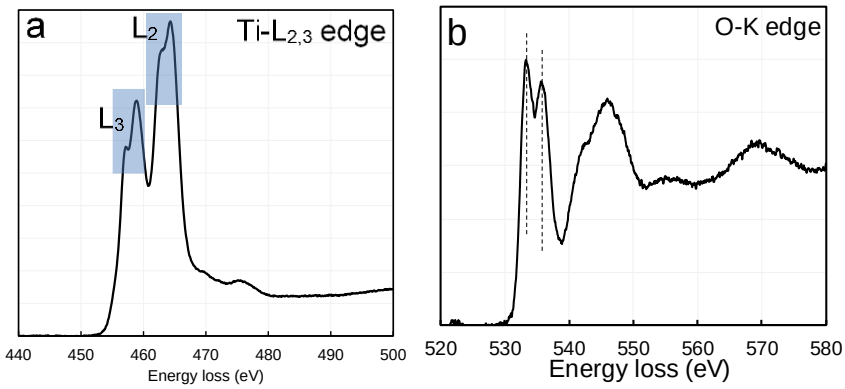


Figure S4. The Ti-$L_{2,3}$ (a), and O-K edge (b) EEL spectra of oxidized $Ti_3C_2T_x$ flakes.

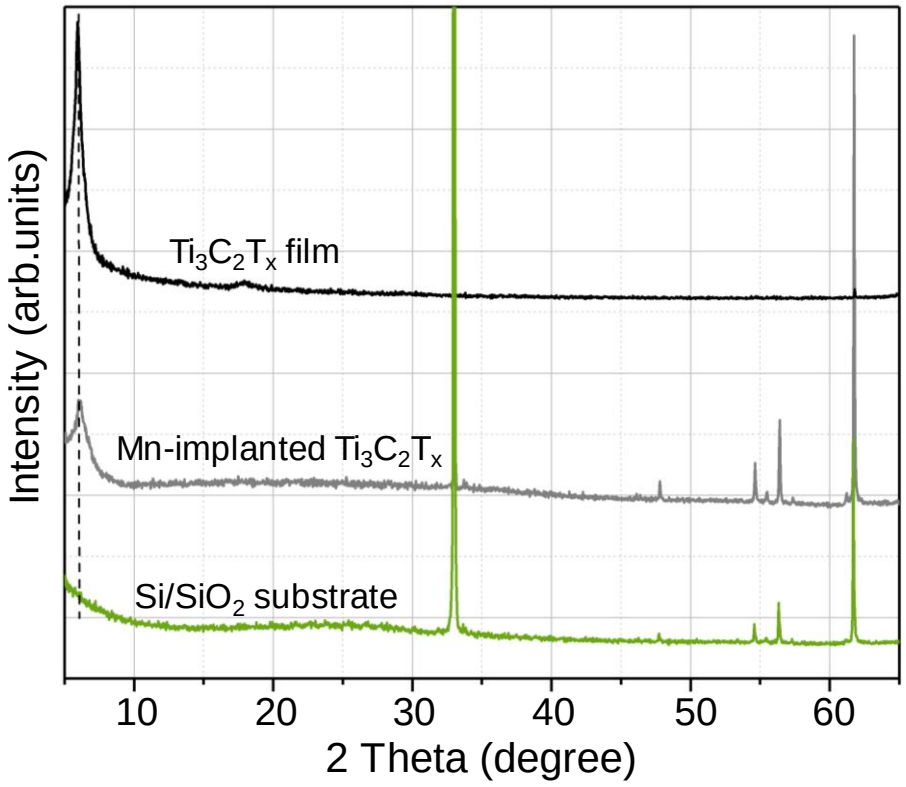


Figure S5. XRD patterns of the $Ti_3C_2T_x$ spin-coated film before implantation (black curve), $Ti_3C_2T_x$ films implanted with $1 \cdot 10^{15}$ Mn-ions/cm^2 at 60 keV (grey curve). The bottom curve shows, for comparison, the XRD pattern of the Si/SiO_2 substrate (green curve).

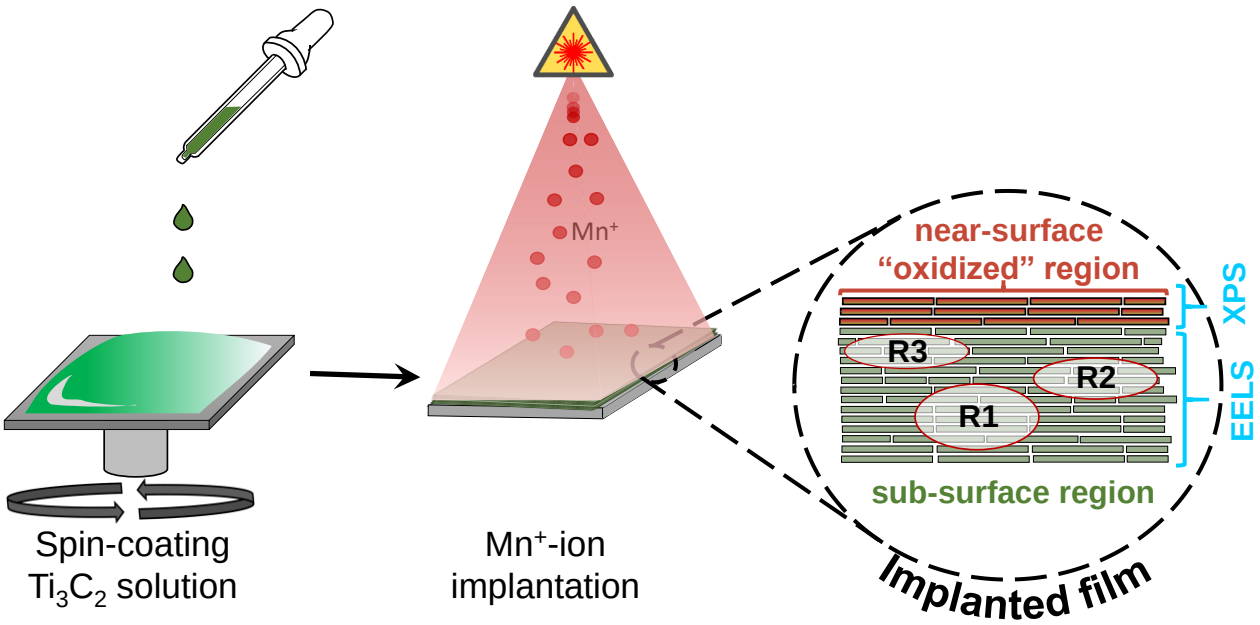
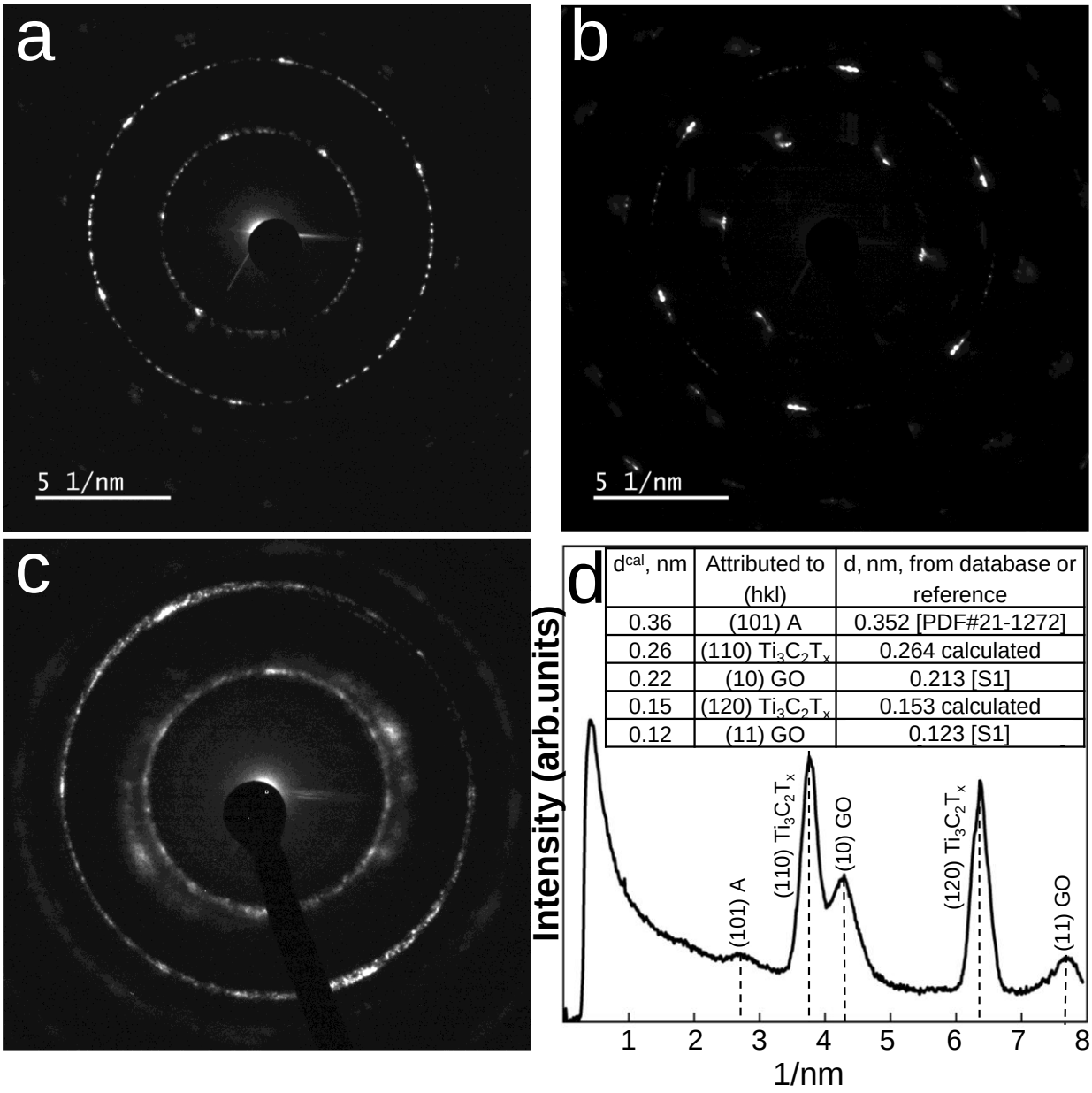


Figure S6. Schematic description of the ion implantation procedure and the implanted film “structure”, showing different regions labeled as R1-R3, used to perform electron energy loss spectroscopy analysis of implanted with $1 \cdot 10^{16}$ Mn-ions/cm^2 $Ti_3C_2T_x$ film. The R1-R3 regions are given for a schematic illustration. The precise position of the R1-R3 fragments in the film have not been determined.



d^{cal}, nm	Attributed to (hkl)	d, nm, from database or reference
0.36	(101) A	0.352 [PDF#21-1272]
0.26	(110) $Ti_3C_2T_x$	0.264 calculated
0.22	(10) GO	0.213 [S1]
0.15	(120) $Ti_3C_2T_x$	0.153 calculated
0.12	(11) GO	0.123 [S1]

Figure S7. SAED patterns of studied **R1** (a), **R2** (b), and **R3** (c) regions extracted from different parts of sub-surface region (**Figure S5**) of $1 \cdot 10^{16}$ ions/cm^2 Mn-implanted $Ti_3C_2T_x$ film. (d) The radial intensity profile of the R3 region SAED pattern presented in (c). d-spacing values, d^{cal}, are calculated from experimental SAED patterns (a, b, insets). Reference values of d-spacings for anatase (A) were taken from JCPDS database – PDF#21-1272. Reference values of d-spacings for graphene oxide (GO) were taken from the Reference S1.

REFERENCES

S1 Wilson, N.; Pandey, P.A.; Beanland, R.; Rourke, J.P.; Lupo, U.; Rowlands, G.; Roemer, R.A. On the Structure and Topography of Free-Standing Chemically Modified Graphene. *New J. Phys.* **2010**, *12*, 125010.