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Supplementary Materials for

Pressure-induced shear and interlayer expansion in Ti₃C₂ MXene in the presence of water

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- fig. S3. Analysis of material ejected from the side of the die.

Supplementary Materials



fig S1. Full diffraction pattern of $Ti_3C_2T_x$ compressed in excess H₂O at a pressure of 2 GPa. The asterisk denotes the (002) peak of a small amount of Ti_3AlC_2 impurity. Open circles denote reflections from the MXene $Ti_3C_2T_x$, in order from left to right: {00*l*}, (011), (013), (015), (016), (017). Lines represent the standard of D₂O Ice VI; the experimental peaks are shifted to higher angle because the standard is at 1.1 GPa and the experimental pattern is at 2 GPa. JCPDS standard for Ice-VI (#086-16531; 225K, 1.1GPa). Ice-VI reflections are indexed.



fig S2. Full diffraction pattern of $Ti_3C_2T_x$ compressed in excess H₂O at a pressure of 3 GPa. The asterisk denotes the (002) peak of a small amount of Ti_3AlC_2 impurity. Open circles denote reflections from the MXene $Ti_3C_2T_x$, in order from left to right: {00*l*}, (011), (013), (015), (016), (017). Lines represent the standard of D₂O Ice VII; the experimental peaks are shifted to higher angle because the standard is at 2.6 GPa and the experimental pattern is at 3 GPa. JCPDS standard for Ice-VII (#085-1391; 296K, 2.6GPa). Ice-VII reflections are indexed.



fig S3. Analysis of material ejected from the side of the die. (A) Schematic showing the setup of disc pressing in a steel die with 3-part walls. The large arrows indicate the direction of the uniaxial pressure, and the small arrow shows the location of MXene collected that was ejected from the main pressing area and up along the inside of the die walls. The MXene disc is shown in dark grey at the center. (B) XRD of the same material, showing the same expansion as observed on the surface of the disc. (C) SEM image of the collected material, showing large areas with nanosheets that have slipped relative to each other into a turbostratically-disordered surface.