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Supplementary Information for

Mo_2Ga_2C: a new ternary nanolaminated carbide

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S1 Experimental Details:

a. Synthesis of the bulk Mo_2Ga_2C:

The starting materials used were commercial Mo (63 NS, Metco Inc., Anderson, SC), graphite (Grade 4827, Asbury Graphite Mills Inc., Asbury, NJ) powders and Ga shots (99.99%) (Roto Metals Inc., San Leandro, CA). First the Mo and graphite powders were weighed in a 2:1 molar ratio and placed in a plastic bottle and mixed for 24 h using agate balls as the milling media. The resulting, lightly sintered, Mo_2C compact was crushed into powder and mixed with Ga in a 1:8 molar ratio to form Mo_2Ga_2C. The mixture was then placed in a quartz tube that was evacuated using a mechanical vacuum pump and sealed. The latter was then placed in an alumina tube furnace and heated at a rate of 10 °C/min to 850 °C, and held at that temperature for 48 h. After furnace cooling, the powder was immersed in a 37 wt. % HCl solution for 3 days to dissolve any residual Ga and Ga_2O_3 if present. Predominantly single phase Mo_2Ga_2C powder – with ≈ 20 wt.% Mo_2C– was obtained. The powders were then washed with deionized water several times and dried in air for further analysis.

b. Thin film synthesis:

Direct current magnetron sputtering was used to grow Mo-Ga-C thin films were synthesized. The films were co-deposited from three elemental targets, Mo (3-inch, 99.95% purity, SCOTECH Ltd.), Ga (2-inch, 99.99999% purity, 5N Plus UK Ltd.) and C (3-inch, 99.99% purity, SCOTECH Ltd.) with respective powers 40 W, 18 W and 200 W and at ~0.5 Pa Ar with a background pressure in the range of 10^{-7} Pa. Due to its low melting point (~ 30°C), the Ga source was kept in a concave stainless steel crucible right below the substrate, in line with previously developed procedures. [A. Petruhins, A. S. Ingason, M. Dahlqvist, A. Mockute, M. Junaid, J. Birch, J. Lu, L. Hultman, P. O. Å. Persson and J. Rosen, Phys. Status Solidi RRL, vol. 7, no. 11, pp. 971-974, 2013]. The Mo and C targets were tilted +35° and -35° away from the horizontal position of the Ga target, co-focusing onto the rotating substrate.

The thin films were grown on MgO(111) substrates (10×10×0.5 mm^3, Latech Ltd.) that were ultrasonically cleaned sequentially in acetone, ethanol and isopropanol for 10 minutes at each stage. Before deposition, the substrate was heated to 560 °C at the base pressure, followed by a 10 minutes pre-sputtering with the same powers used for deposition. A shutter was inserted to blind the substrate from the target's line-of-sight when pre-sputtering, and was afterwards removed directly to start the deposition at the same substrate temperature set-point (560°C).

S2 Characterization Details:

a) Details of XRD Experimental Parameters and Refinement Conditions

XRD patterns were obtained with a diffractometer (Rikagu Smartlab, Tokyo, Japan), with a step size of 0.02° in the 3°-120° 2 theta range with a step time of 7 s with a 10x10 mm^2 window slit. Scans were made with Cu-Kα radiation (40 kV and 44 mA).

Rietveld refinement of the XRD diffractograms was carried out using the FULLPROF code [J. Rodrıguez-Carvajal, Phys. B 192 (1993) 55–69]. The refinement was carried out from 8.5° to 120° 2θ. Refined parameters were: five background parameters, scale factors from which relative phase fractions are evaluated, *Y* profile parameter for peak width, lattice parameters (LPs), the overall thermal factor, preferred orientation and atomic positions for all phases. The experimental and those calculated from the Rietveld refinement are summarized in Table S1.

Table S1: X-ray (Cu Kα) powder diffraction data for Mo_2Ga_2C.

Peak Number	h	k	l	2theta	I calculated	I observed	d-hkl
1	0	0	2	9.775	440.1	460.1	9.040678
2	0	0	4	19.623	12.9	0	4.520339
3	0	0	6	29.619	8.7	0	3.013559
4	1	0	0	34.095	639.6	646.7	2.627484
5	1	0	1	34.465	87.6	79.1	2.600175
6	1	0	2	35.552	4.6	15.7	2.523087
7	1	0	3	37.303	1439.2	1607.4	2.408563
8	1	0	4	39.644	22.3	31.1	2.271614
9	0	0	8	39.853	480.5	513.7	2.26017
10	1	0	5	42.493	1128.4	1308.5	2.125649
11	1	0	6	45.779	16.4	83.9	1.980435
12	1	0	7	49.44	91.9	86.8	1.842001
13	0	0	10	50.43	3.1	0	1.808136
14	1	0	8	53.43	361.3	375.3	1.713455
15	1	0	9	57.718	0.3	0	1.595959

Peak Number	h	k	l	2theta	I calculated	I observed	d-hkl
16	1	1	0	61.032	530.3	492.5	1.516979
17	0	0	12	61.49	14.2	12.1	1.50678
18	1	1	2	61.979	20.9	20.1	1.496064
19	1	0	10	62.282	7.1	5.8	1.489519
20	1	1	4	64.771	4.4	1.3	1.438156
21	1	0	11	67.114	174	128.1	1.393528
22	1	1	6	69.29	6.6	16.4	1.354988
23	2	0	0	71.795	68.6	56.8	1.313742
24	2	0	1	72.014	8.5	7.2	1.310288
25	1	0	12	72.217	7.8	6.3	1.307101
26	2	0	2	72.668	1	1	1.300087
27	0	0	14	73.228	2	1.6	1.291525
28	2	0	3	73.755	185.1	165.8	1.283603
29	2	0	4	75.265	2.7	2.5	1.261544
30	1	1	8	75.404	432.9	431.9	1.259573
31	2	0	5	77.193	185.9	182.1	1.234785
32	1	0	13	77.604	181.9	193.4	1.229266
33	2	0	6	79.529	3.4	4.6	1.204282
34	2	0	7	82.267	17.9	24.4	1.17099
35	1	1	10	83.031	5.5	9	1.162145
36	1	0	14	83.3	0.9	1.5	1.159069
37	2	0	8	85.405	90.3	89.9	1.135807
38	0	0	16	85.942	46.6	49.1	1.130085
39	2	0	9	88.945	0.2	0.1	1.099527
40	1	0	15	89.347	26.2	18.9	1.095625
41	1	1	12	92.199	28.2	34.5	1.069042
42	2	0	10	92.898	2.8	3.7	1.062824
43	1	0	16	95.804	48.9	45.5	1.038136
44	2	0	11	97.284	74.5	80.4	1.026246
45	0	0	18	100.14	1.4	5.9	1.00452
46	2	1	0	101.728	63.2	69.1	0.993096
47	2	1	1	101.941	5.5	5.8	0.991601
48	2	0	12	102.138	3.7	4.2	0.990218
49	2	1	2	102.579	1.6	2.2	0.987158
50	1	0	17	102.762	5.5	7.5	0.985896
51	1	1	14	103.128	8.9	10	0.983394
52	2	1	3	103.647	190.3	177	0.979883
53	2	1	4	105.15	2.8	2.3	0.969963
54	2	1	5	107.098	211.4	218.3	0.957642
55	2	0	13	107.519	104.8	111.9	0.95506

Peak Number	h	k	l	2theta	I calculated	I observed	d-hkl
56	2	1	6	109.508	5.6	16.2	0.943201
57	1	0	18	110.362	0.8	5.4	0.938286
58	2	1	7	112.403	19.4	37	0.926948
59	2	0	14	113.517	1.1	2.6	0.921001
60	2	1	8	115.822	132.4	125.5	0.9092
61	1	1	16	109.508	5.6	16.2	0.943201
62	0	0	20	110.362	0.8	5.4	0.938286
63	1	0	19	112.403	19.4	37	0.926948
64	2	1	9	113.517	1.1	2.6	0.921001

b) TEM, XRD and Structural Characterization

The TEM specimens were prepared by mechanic polishing followed by ion thinning down to electron transparency. High resolution scanning electron microscopy (HRSTEM) and X-ray energy dispersive spectroscopy (EDX) were performed with a double Cs corrected FEI Titan3 60–300 operated at 300 kV, equipped with the Super-X EDX system. Selected area electron diffraction (SAED) characterization was carried out using a FEI Tecnai G2 TF20 UT instrument operated at 200 kV with a point resolution of 0.19 nm. Structural characterization of the thin films was performed through X-ray diffraction (XRD). The system utilized was a Panalytical Empyrean MRD with a Cu k_α source. The measurements performed were symmetric (θ-2θ) scans obtained by employing a hybrid mirror and a 0.27º parallel plate collimator in the incident and the diffracted beam side, respectively.

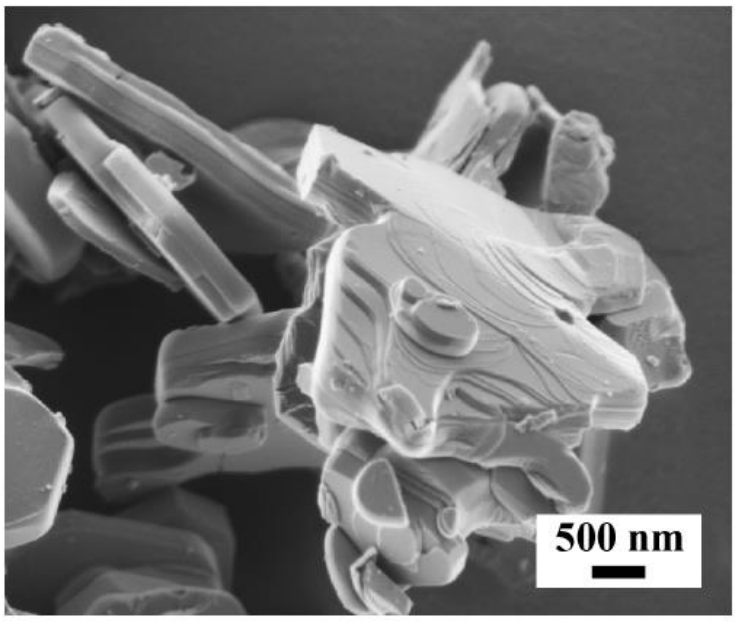

Fig. S1 Scanning electron microscope micrograph of Mo_2Ga_2C powders showing typical MAX phase platelet morphology.

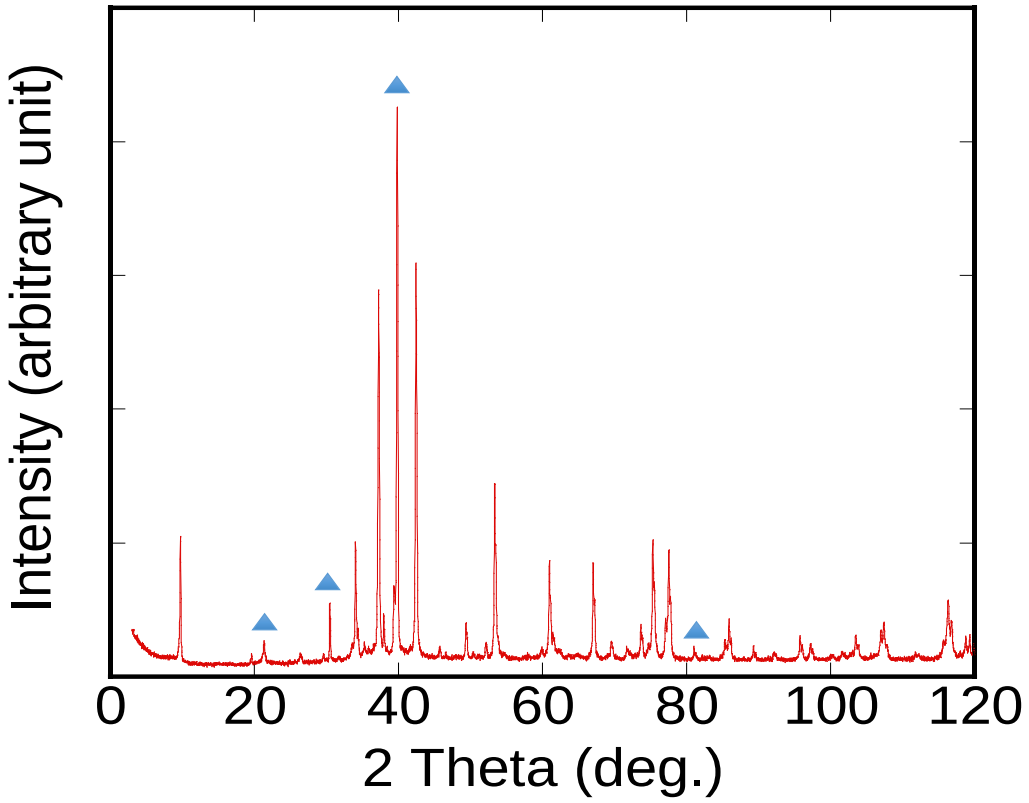

Fig. S2 XRD pattern of Mo2Ga2C bulk sample, the triangle markers represent peaks for free Gallium.