Direct MoB MBene domain formation in magnetron sputtered MoAlB thin films

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Supplementary data

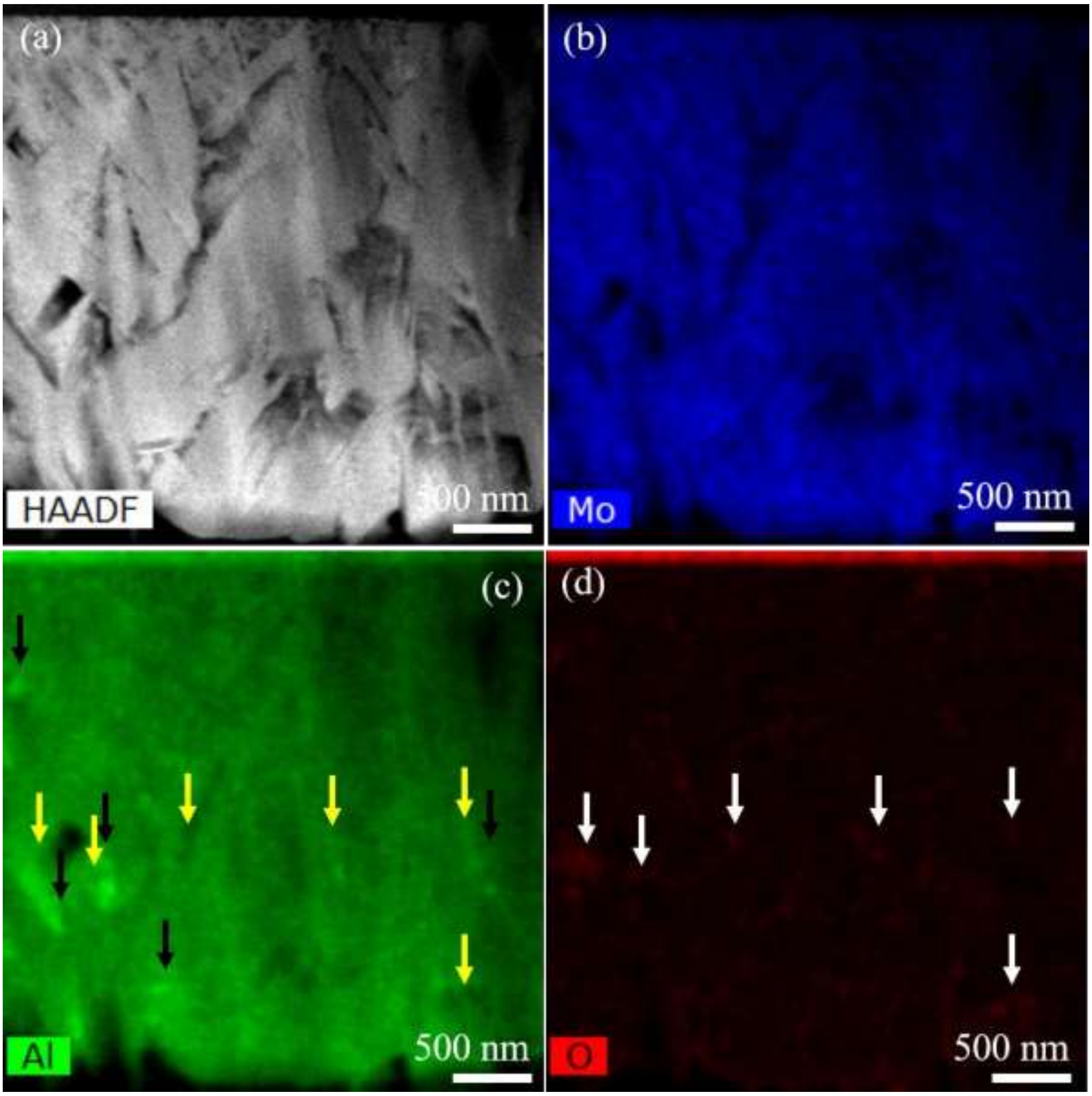

Figure S1: (a)-(d) Large-scale STEM EDX showing chemical composition mapping of Mo, Al and O. Al-rich and O-rich phases are marked by black and white arrows in (c) and (d) respectively. Representative areas of AlO_X are marked by yellow arrows in (c).

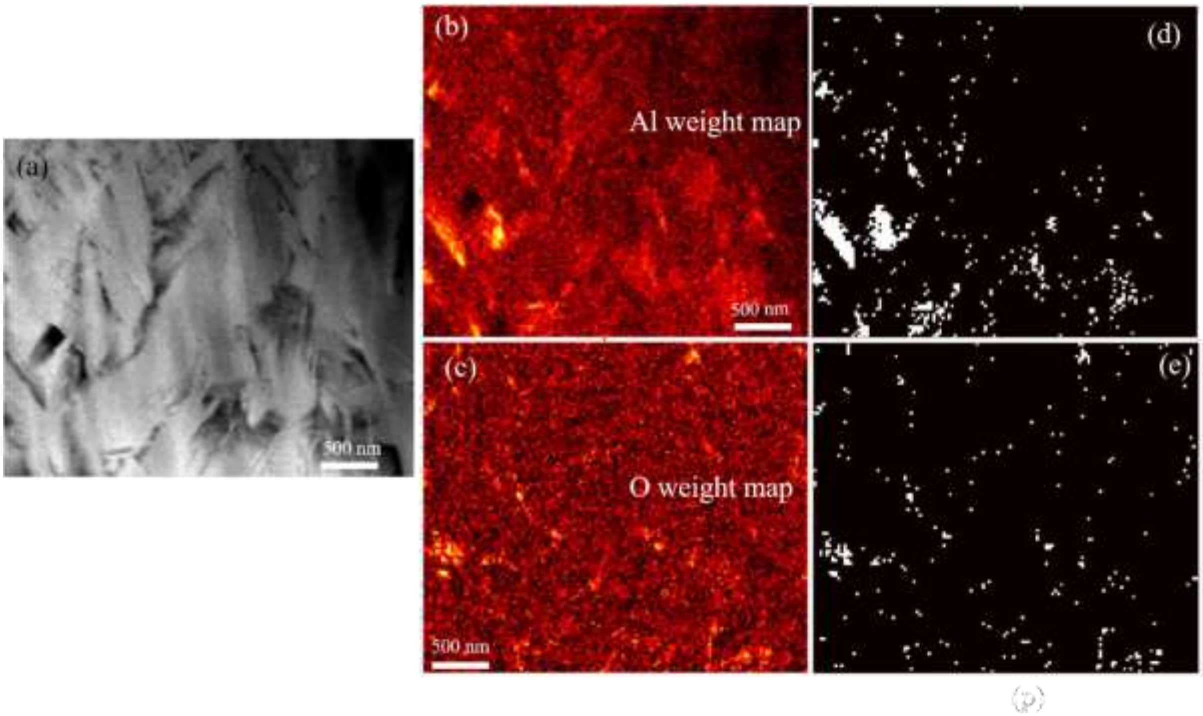

Figure S2: (a) HAADF STEM image of MoAlB (part of the area as shown in S1). (b)-(c) EDX weight mappings processed by multivariate statistical analysis [S1] for the Al-rich (b) and O-rich phases (c). Areas of Al-rich (**d**) and O-rich (**e**) phases are highlighted in white. The area fractions of the Al-rich and O-rich phases are 4.5% and 2%, respectively.

Time-of-flight elastic recoil detection analysis (ToF-ERDA)

Time-of-flight elastic recoil detection analysis (ToF-ERDA) was performed at the tandem accelerator laboratory of Uppsala University, Sweden, using 36 MeV $^{127}I^{8+}$ primary ions. Details can be found in [S2]. Reference measurements on bulk borides were used to estimate the total uncertainty of < 5% relative. This uncertainty is governed by the systematic uncertainty of stopping powers from primary ions as well as the recoiling particles as discussed in the supplementary material of [S3].

The chemical composition depth profiling by ToF-ERDA revealed a chemical composition of 29.8 ± 1.5 at.% Mo, 31.2 ± 1.6 at.% Al, 35.1 ± 1.8 at.% B and 3.9 ± 0.2 at.% O within the MoAlB film up to a depth of approximately 100 nm. In addition, locally enriched regions were identified with up to 39.7 ± 2.0 at.% Al and 24.7 ± 1.2at. % O, while the Mo and B concentrations were reduced to 14.7 ± 0.7 and 20.9 ± 1.0 at.%, respectively. The data are summarized in table S1 and compared to the values of the film deposited with two targets (ref. 23 in the manuscript). Due to the large measurement spot of approximately 2×1 mm it is reasonable to assume that MoAlB as well as AlO_x phases co-exist in the probed volume.

Elemental Composition % at.	Mo	Al	B	O	
Using two targets: MoB & Al	29.4±3.2	31.5±3.5	34±4	5±1	Ref. [23]
Using single target: MoAlB	29.8±1.5	31.2±1.6	35.1±1.8	3.9±0.2	This work

Table S1: Average composition of the MAB phase as deduced by ToF-ERDA.

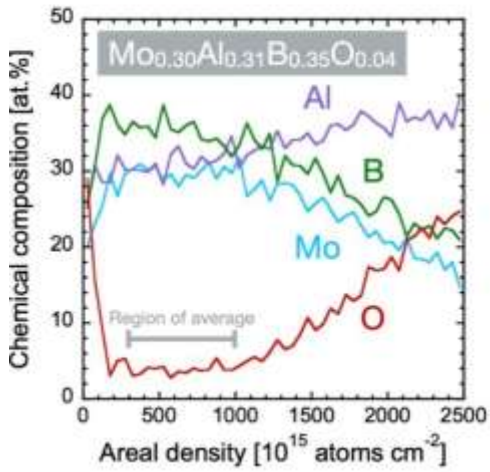

Figure S3: Chemical composition depth profile as obtained from ToF-ERDA. The region used to obtain the average composition of the MAB phase is indicated in grey.

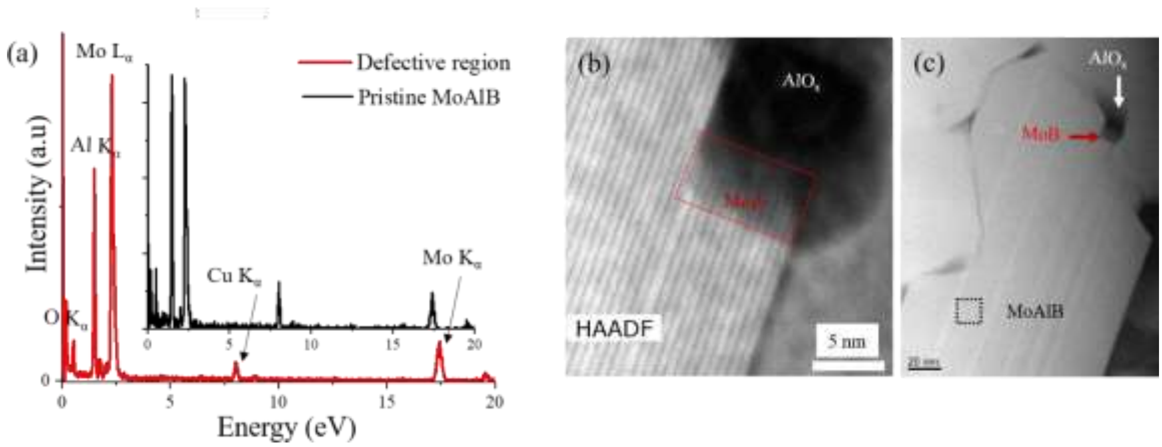

Figure S4: (a) Comparison of EDS spectra and Mo and Al intensities in MoAlB and MoB region. HAADF images (b) and (c) where the areas of spectra acquisition for MoB (red rectangle) and MoAlB (black rectangle) are marked.

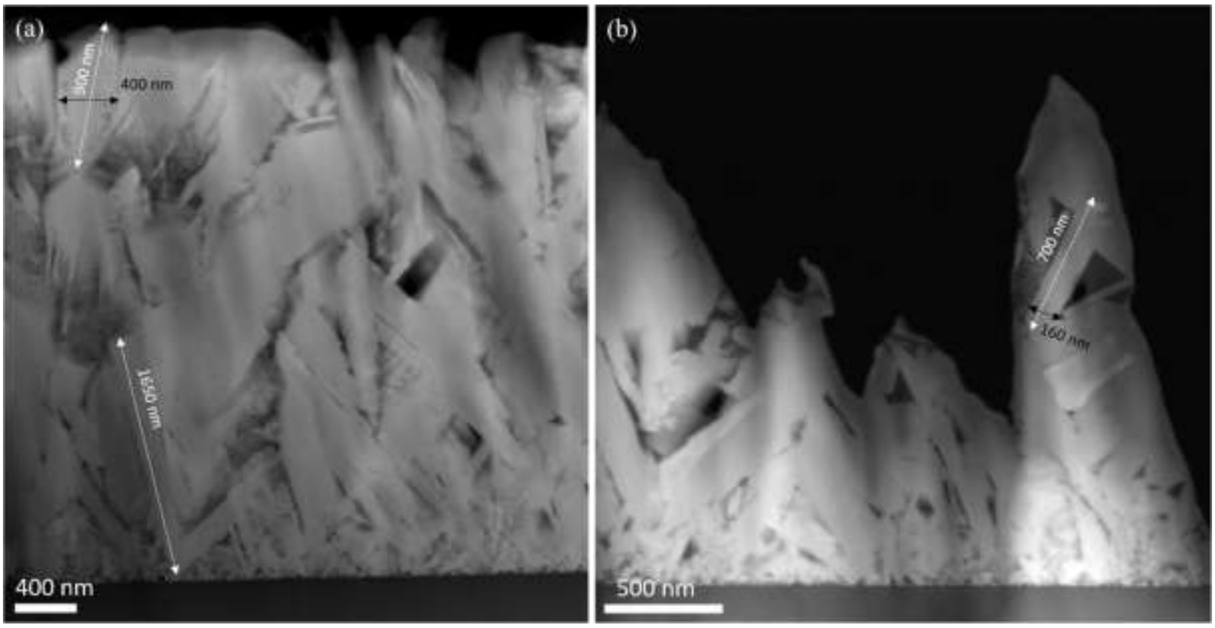

Figure S5: Low magnification HAADF STEM shows an average statistical analysis of MoAlB domain measuring the grain size in (a). The MoAlB grain in (b) is the area of interest described in the manuscript.

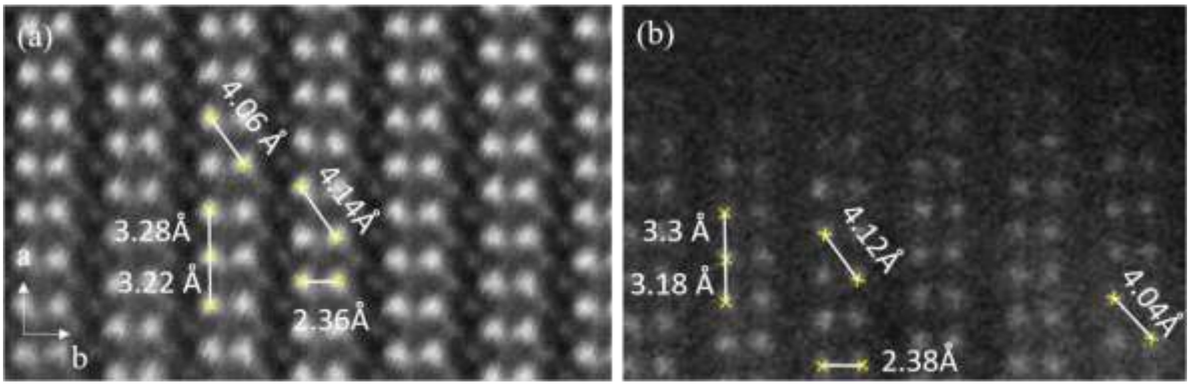

Figure S6: Gauss peak fitting were carried out for (a) MoAlB and (b) MoB region. Yellow crosses mark the center of mass of Mo atoms shown as example. Representative Mo-Mo distance measurements are marked by white lines

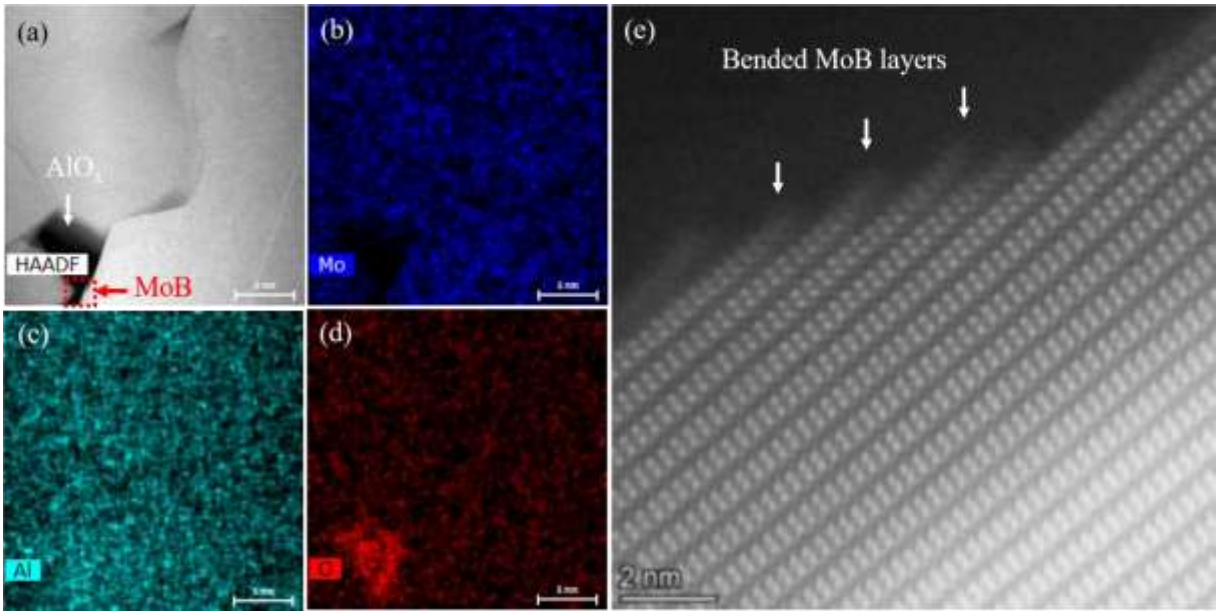

Figure S7: (a) HAADF STEM image where AlO_x region (white arrow) and 2D MoB MBene area (red dotted rectangle) are marked. (b)-(d) are STEM EDS showing chemical mapping of the same area as in (a). (e) HR-STEM image depicting bent MoB layers marked with white arrows.

References

[S1] S. Zhang and C. Scheu, Evaluation of EELS spectrum imaging data by spectral components and factors from multivariate analysis, *Microscopy,* 2017, **67,** i133–i141.

[S2] M. Hans, M. Baben, D. Music, J. Ebenhöch, D. Primetzhofer, D. Kurapov, M. Arndt, H. Rudigier and J. M: Schneider, Effect of oxygen incorporation on the structure and elasticity of Ti-Al-O-N coatings synthesized by cathodic arc and high-power pulsed magnetron sputtering, *J. Appl. Phys.*, 2014, **116,** 093515.

[S3] M. Baben, M. Hans, D. Primetzhofer, S. Evertz, H. Ruess and J. M. Schneider, Unprecedented thermal stability of inherently metastable titanium aluminum nitride by point defect engineering, *Mater. Res. Lett.*, 2017, **5 (3),** 158-169.