Electronic Supplementary Material (ESI) for Nanoscale.

Defects in an orthorhombic MoAlB MAB phase thin film grown at moderate synthesis temperature

Rajib Sahu*[a,b], Dimitri Bogdanovski[b], Jan-Ole Achenbach[b], Jochen M Schneider[a,b] and Christina Scheu*[a,c]

[a]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

[b]Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany

[c]Materials Analytics, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany

*Corresponding authors: r.sahu@mpie.de, c.scheu@mpie.de

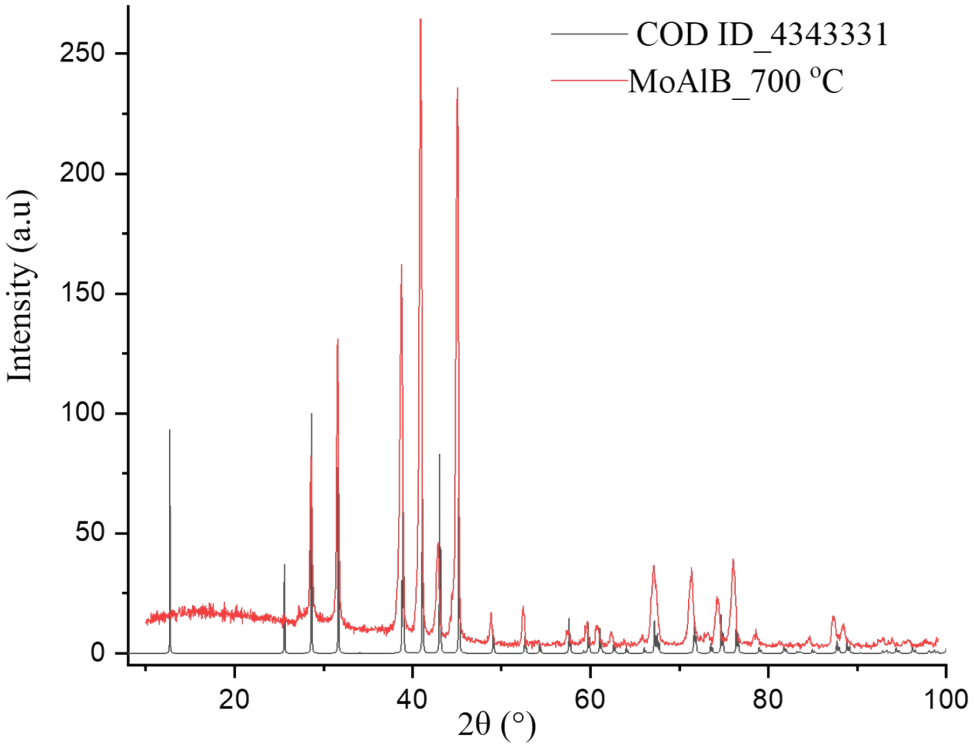

Fig. S1: X-ray diffraction data of the MoAlB film grown by DC magnetron sputtering. Reference pattern and reference card number are taken from Crystallography Open Database [1].

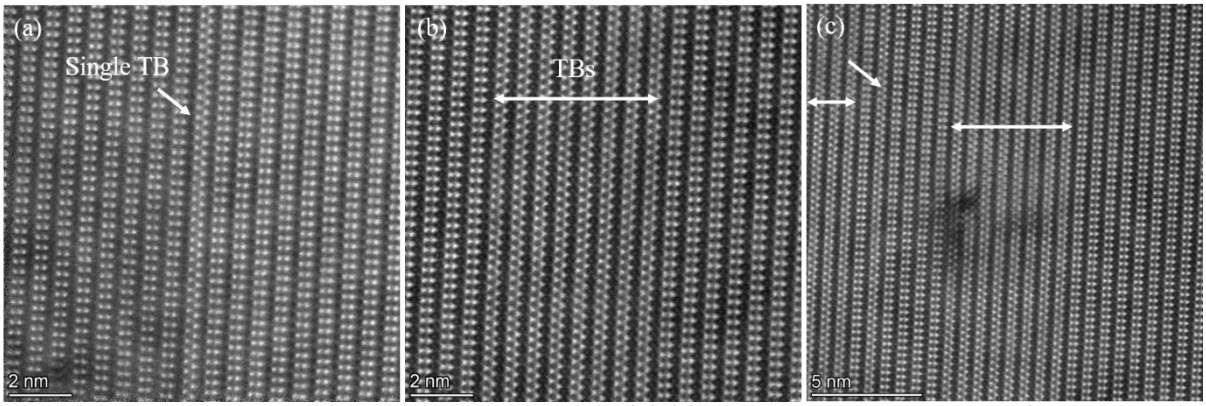

Fig. S2: High resolution HAADF STEM micrographs in (a)-(c) represent single-unit wide (white arrow) to several-nanometer-wide twin domains (double headed arrows) within different grains.

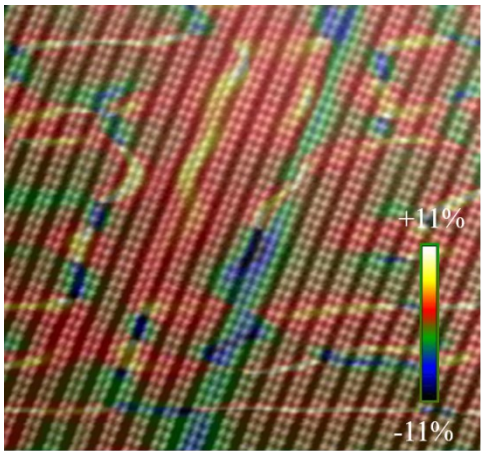

Fig. S3: Local phase map showing relative interplanar differences along ϵ_{yy} .

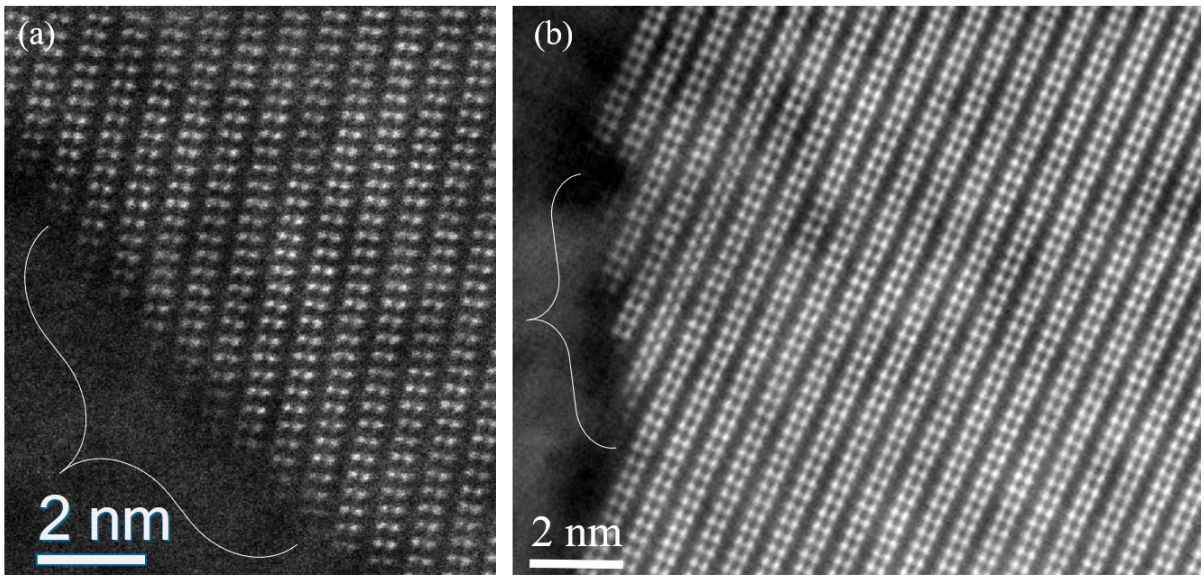

Fig. S4: HAADF STEM micrographs showing faceted grain boundaries from two different areas (a) and (b).

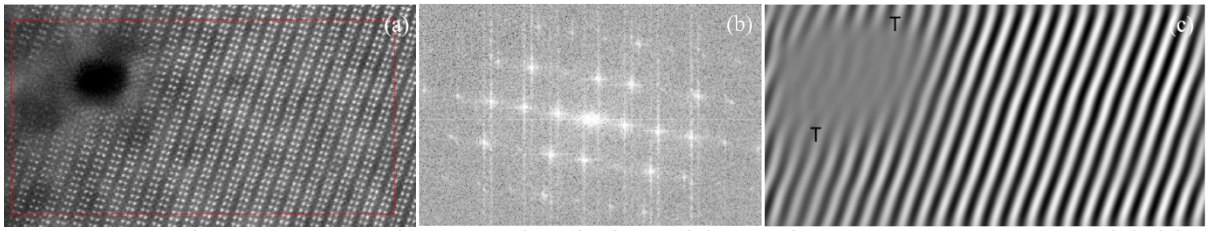

Fig. S5: Inverse fast Fourier transformation (IFFT) of area (a) is performed using FFT image in (b). (c) Lattice fringes over the 3D amorphous region show a discontinuity.

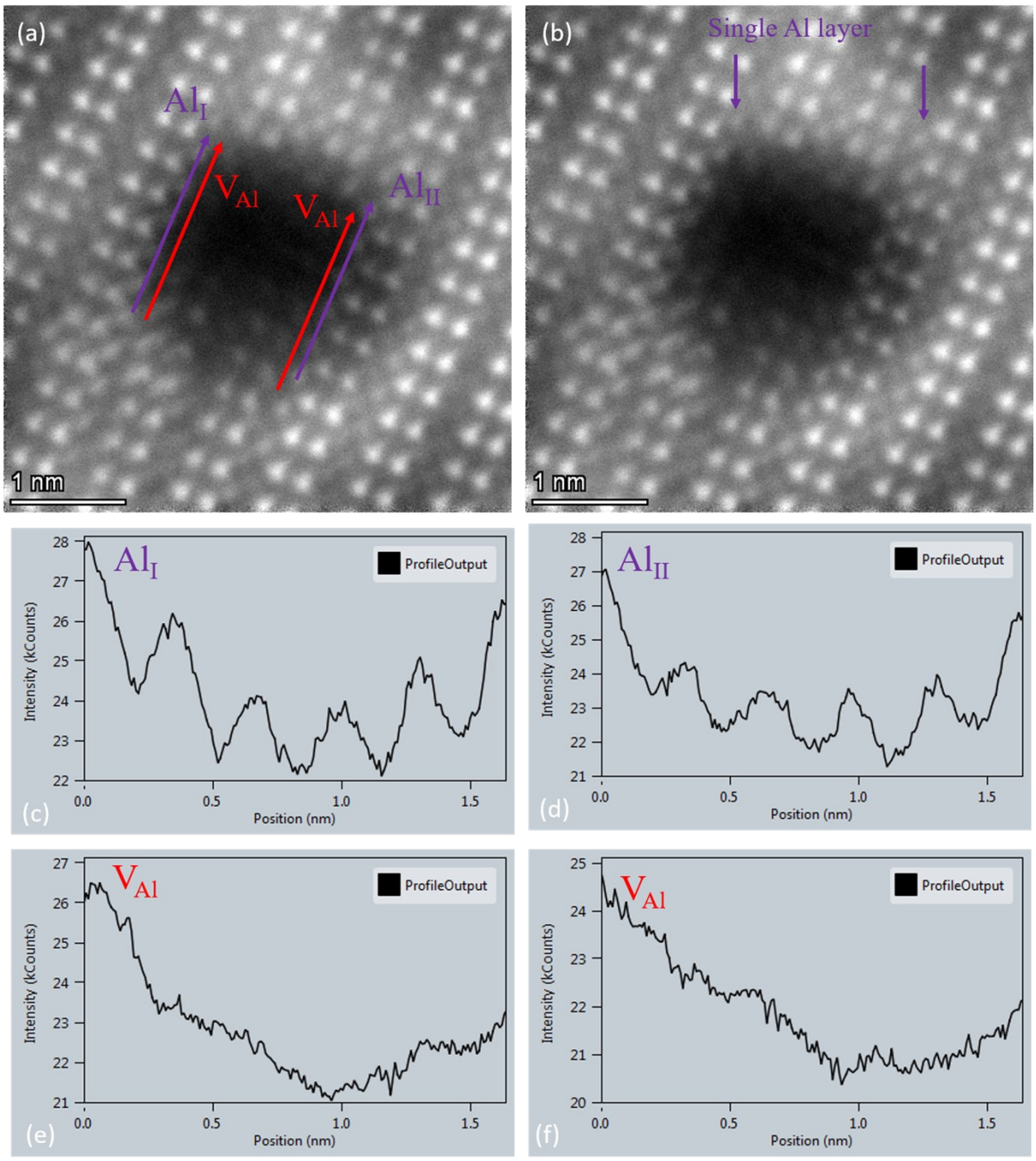

Fig. S6: (a) Presence of single-layer Al at the vicinity of the 3D cluster is denoted by Al_I and Al_{II} and the vacant columns are marked by V_{Al}. Corresponding line profile are drawn in (c)-(f). Al atoms in single layer are indicated by violet arrows in the HAADF STEM micrographs (b).

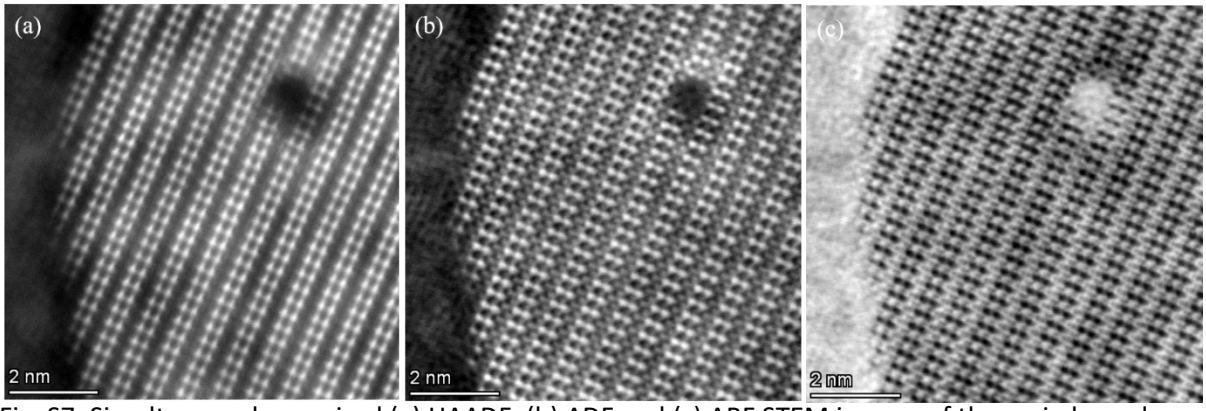

Fig. S7: Simultaneously acquired (a) HAADF, (b) ADF and (c) ABF STEM images of the grain boundary are shown here.

References

1. M. Ade and H. Hillebrecht, Ternary Borides Cr_2AlB_2, Cr_3AlB_4, and Cr_4AlB_6: The First Members of the Series $(CrB_2)_nCrAl$ with n = 1, 2, 3 and a Unifying Concept for Ternary Borides as MAB-Phases, *Inorg. Chem.,* 2015, **54**(13), 6122-6135.