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Imaging of ALD Grown W Atoms on α-TiO2(110) by X-ray Standing Wave Fourier Inversion CHANG-YONG KIM, Northwestern University, JEFFREY ELAM, MICHAEL PELLIN, Argonne National Laboratory, DIPAK GOSWAMI, STEVEN CHRISTENSEN, MARK HERSAM, PETER STAIR, MICHAEL BEDZYK, Northwestern University — Supported metal oxides are among the most important of catalytic materials systems. However, there is a lack of experimental atomic-scale structural information for describing the relevant interfaces. We combine atomic layer deposition (ALD) and x-ray standing wave (XSW) atomic-imaging to address this challenge. As a first case, we determine the precise registry of W atoms on a rutile TiO2(110) surface. The ALD W layer was formed by first exposing the TiO_2 surface to disilane (Si_2H_6) and then to tungsten hexafluoride (WF_6). The direct-space image reveals that W occupies the Ti-site that would be occupied by Ti if the bulk structure were extended above surface. The tungsten atoms are vertically shifted upward from the ideal Ti-site location by +0.23 Å. These XSW measurements of ALD heterolayer growth clearly show for the first time that ALD conformal layers can be highly coherent with the substrate lattice. The ALD method for supported catalyst material preparation provides a bridge over the "materials preparation gap" that typically separates practical, high-surface-area and single crystal model catalytic materials.

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