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Grains and grian boundaries in highly-crystalline monolayer molybdenum disulfide AREND M. VAN DER ZANDE, Energy Frontier Research Center, Columbia University, PINSHANE Y. HUANG, Cornell University, DANIEL A. CHENET, YUMENG YOU, TIMOTHY C. BERKELBACH, GWAN-HYOUNG LEE, DAVID R. REICHMAN, Columbia University, DAVID A. MULLER, Cornell University, TONY F. HEINZ, JAMES C. HONE, Columbia University — Recent progress in large-area chemical vapor deposition (CVD) synthesis of monolayer molybdenum disulfide, a new two-dimensional direct-bandgap semiconductor, is paving the way for applications in atomically thin electronics. Little is known, however, about the microstructure of this material. Here we have refined CVD synthesis to grow highly crystalline islands of monolayer molybdenum disulfide up to 120 micrometers in size with optical and electrical properties comparable or superior to exfoliated samples. Using transmission electron microscopy, we correlate lattice orientation, edge morphology, and crystallinity with island shape to demonstrate that triangular islands are single crystals. The crystals merge to form faceted tilt and mirror boundaries that are stitched together by lines of 8- and 4- membered rings. Density functional theory reveals localized mid-gap states arising from these 8-4 defects. The knowledge gained about grain structure enables systematic studies of the optical, mechanical, and electronic properties of grain boundaries.

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