

Supporting information:

Temperature-Driven Twin Structure Formation and Electronic Structure of Epitaxially Grown Mg_3Sb_2 Films on Mismatched Substrates

Sen Xie ^{1,2,†}, Yujie Ouyang ^{1,2,†}, Wei Liu ^{1,*}, Fan Yan ¹, Jiangfan Luo ¹, Xianda Li ¹, Ziyu Wang ³, Yong Liu ^{4,*} and Xinfeng Tang ^{1,*}

¹ State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Wuhan 430070, China

² International School of Materials Science and Engineering, Wuhan University of Technology, Wuhan 430070, China

³ The Institute of Technological Sciences, Wuhan University, Wuhan 430072, China; zywang@whu.edu.cn

⁴ School of Physics and Technology and The Key Laboratory of Artificial Micro- and Nano-Structures of Ministry of Education, Wuhan University, Wuhan 430072, China

* Correspondence: w.liu@whut.edu.cn (W.L.); yongliu@whu.edu.cn (Y.L.); tangxf@whut.edu.cn (X.T.)

† These authors contributed equally to this work.

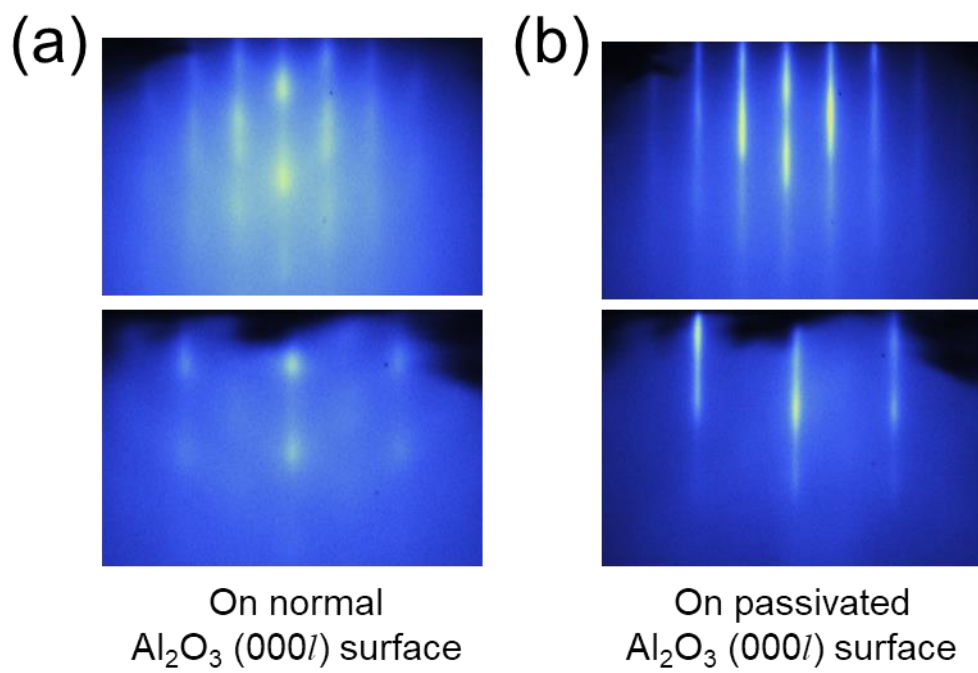


Figure S1. The RHEED patterns of Mg_3Sb_2 films grown on Al_2O_3 (0001) substrates with and without passivation treatment.

The RHEED patterns of Mg_3Sb_2 grown on different substrates

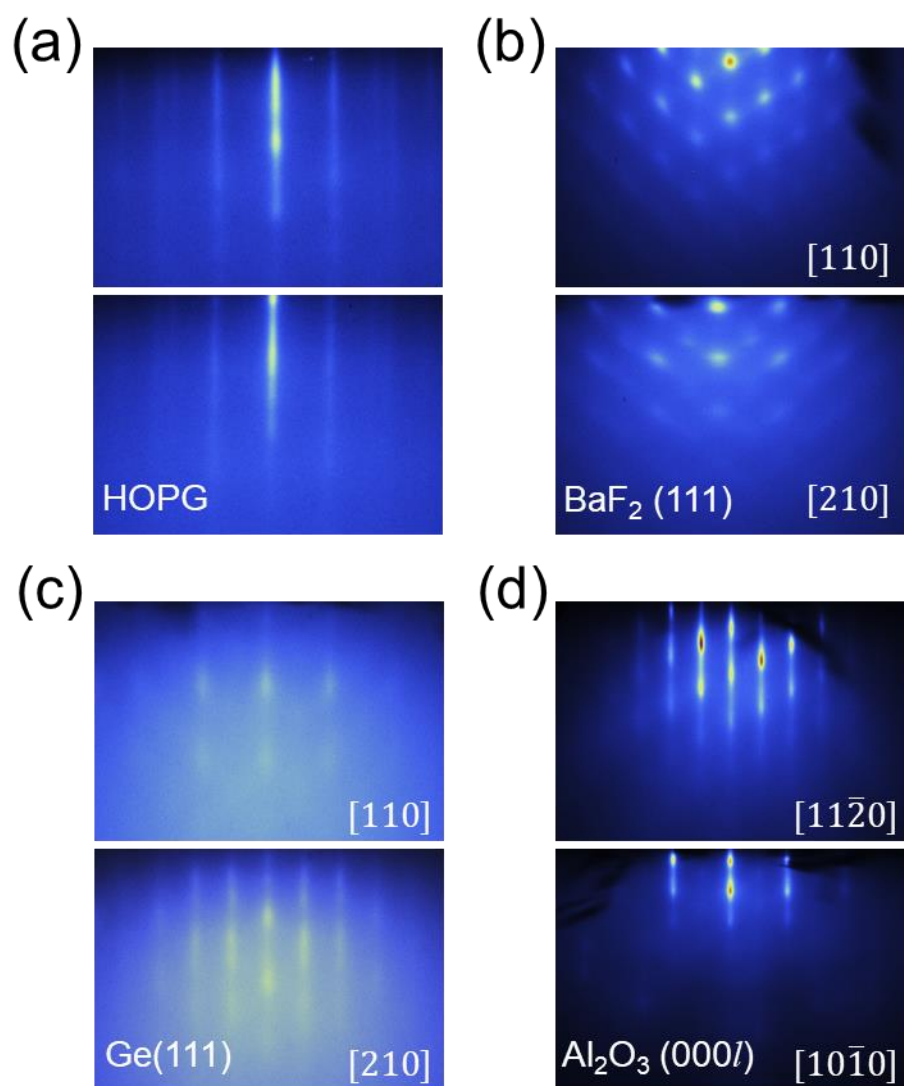


Figure S2. The RHEED patterns of Mg_3Sb_2 grown on different substrates: (a) cleaved HOPG, (b) BaF_2 (111), (c) Ge (111), and (d) Al_2O_3 (000l) substrates. The Mg_3Sb_2 grown on Al_2O_3 shows the highest crystallinity.

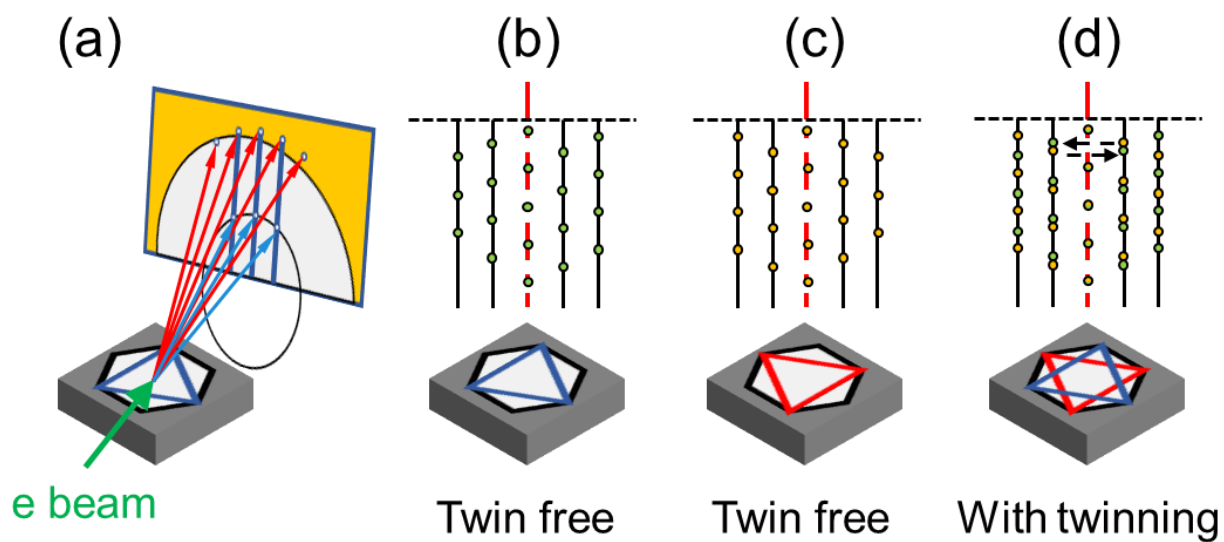


Figure S3. (a) Schematic illustration of the RHEED measurement. (b-d) RHEED patterns of hexagonal lattice with and without twin domains.

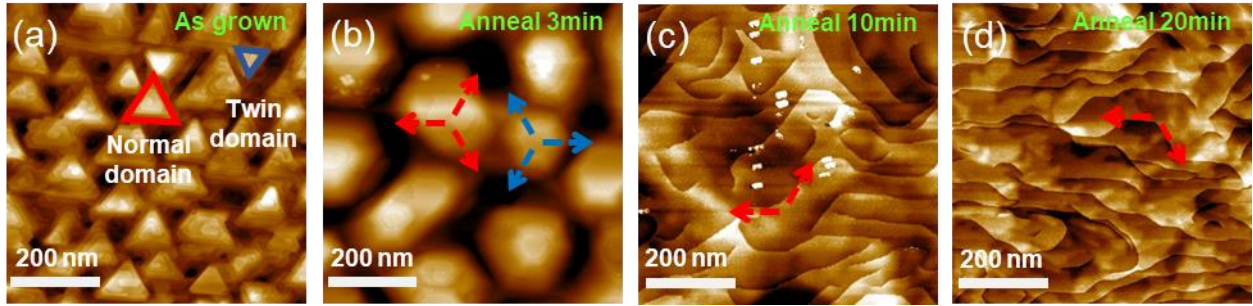


Figure S4. STM surface morphology and structure evolution of Mg_3Sb_2 films grown at 773 K: (a), as-grown; (b), annealed for 3 mins; (c), annealed for 10 mins; (d), annealed for 20 mins. Twin domains are marked by blue triangles in (a) and blue arrows in (b). Annealing at 773 K significantly promotes the crystallinity of films, which is evident from the prominent layer structure and increased grain size.

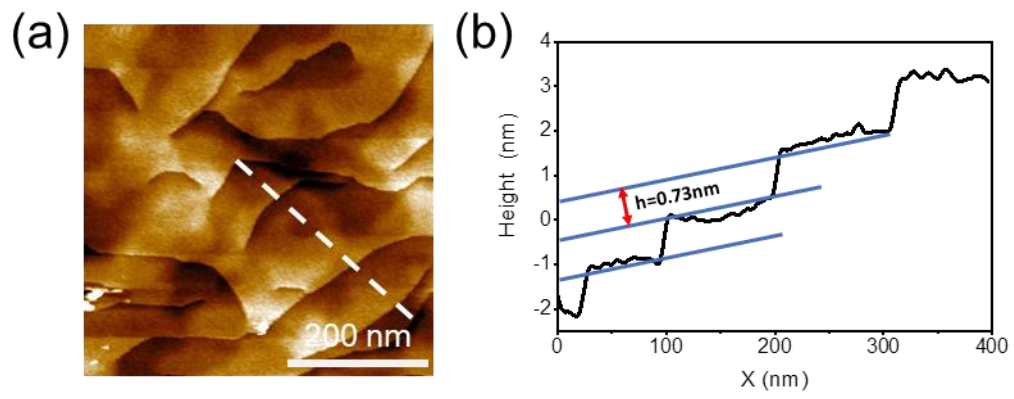


Figure S5. Layer structure of the Mg_3Sb_2 film grown at 773 K and annealed at 773 K for 20 mins: (a) STM surface morphology, (b) The height profile along the white dashed line in (a). The thickness of a single layer is ~ 0.7 nm, in agreement with the spacing of a single lattice layer.