

Supplementary Material: Experimental Evidence of the Topological Surface States in Mg₃Bi₂ Films Grown by Molecular Beam Epitaxy

Tong Zhou(周侗)^{1,2,3,4,†}, Xie-Gang Zhu(朱燮刚)^{2,4,†}, Mingyu Tong(童明玉)^{5,†}, Yun Zhang(张云)^{2,4},
Xue-Bing Luo(罗学兵)^{2,4}, Xiangnan Xie(谢向男)¹, Wei Feng(冯卫)^{2,4}, Qiuyun Chen(陈秋云)^{2,4},
Shiyong Tan(谭世勇)^{2,4}, Zhen-Yu Wang(王振宇)^{1,3,7,*}, Tian Jiang(江天)^{1,5}, Yuhua Tang(唐玉华)^{1,*},
Xin-Chun Lai(赖新春)^{2,*}, and Xuejun Yang(杨学军)^{1,6}

¹State Key Laboratory of High Performance Computing, College of Computer, National University of Defense Technology, Changsha 410073, P. R. China

²Science and Technology on Surface Physics and Chemistry Laboratory, Jiangyou 621908, Sichuan, China

³National Innovation Institute of Defense Technology, Academy of Military Sciences PLA China, Beijing 100010, P. R. China

⁴Institute of Materials, China Academy of Engineering Physics, Mianyang 621700, Sichuan, China

⁵College of Advanced Interdisciplinary Studies, National University of Defense Technology, Changsha 410073, P. R. China

⁶Academy of Military Sciences PLA China, Beijing 100010, P. R. China

⁷Beijing Academy of Quantum Information Sciences, Beijing, 100084, P.R. China

†These authors contributed equally to this work.

**Corresponding authors. Email: oscarwang2008@sina.com; yhtang62@163.com; laixinchun@caep.cn

METHODS

Sample preparation

The Mg₃Bi₂ films were grown on 2×10 mm 6H-SiC(0001) substrate with epitaxially grown Graphene by MBE. The base pressure was maintained at 3×10⁻¹¹ mbar and the vacuum was better than 2×10⁻¹⁰ mbar during growth. Mg (3N) and Bi (5N) sources were thermally evaporated from standard Knudsen cells. Mg and Bi were kept at 380°C and 540°C and with the flux rate of 0.661Å/s and 0.112Å/s (measured by Quartz crystal micro-balance), respectively. The flux ratio between Mg and Bi should be at least ~5:1 to minimize Mg vacancies and ensure the high quality of the as-grown films. The substrate was kept at 350°C during the growth and the quality of the film was monitored by *in-situ* RHEED.

Measurements

For the ARPES measurements, the spectra are excited by the He I α (21.2 eV) resonance line of a commercial Helium gas discharge lamp. The light is guided to the analysis chamber by a quartz capillary. In virtue of the efficient three-stage differential pumping system, the pressure in the analysis chamber is better than 2.0×10^{-10} mbar during our experiments. A VG Scienta DA30L energy analyzer is used to collect the photoelectrons. Mg₃Bi₂ film with the thickness of 50nm was transferred *in-situ* into the ARPES chamber and measurements were done at 12K. The magneto-transport measurements were performed with the standard four-probe technique using silver paint as contacts by Physical Property Measurement System (PPMS-9). The samples for transport measurements is about 50 nm thick in a rectangular shape (5 mm \times 6 mm) grown on Al₂O₃(0001) substrate.

The detailed fitting procedure on SRB slope

Considering the symmetry of SRB1 and SRB2 around $\bar{\Gamma}$, we fit the band by the equation of $y=a \times |x|+b$, where $|x|$ represent the absolute value of x . From Figure S1 we can see that the SRB band between -0.08~-0.22eV of the energy fits well by $y=-4.908 \times |x|+0.191$, and we thus conclude that the slope of SRB band is $C=\pm 4.91$.

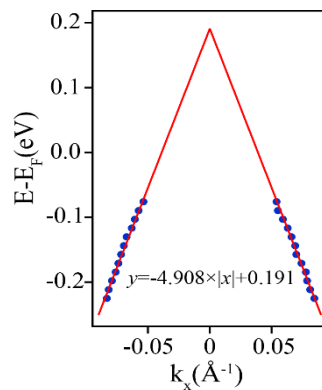


Figure S1. The fitting method for SRB slope. The blue circles indicate SRB band extracting from the MDC peaks and the red line depict the fitting results.

Characterization of Mg₃Bi₂ on Al₂O₃

For magneto-transport measurements, we grew Mg₃Bi₂ films on Al₂O₃(0001) substrate by MBE to exclude the substrate conducting effects. The characterization of Mg₃Bi₂ on Al₂O₃ is shown in Figure S2. The in-plane lattice constant of Al₂O₃ is 4.758 Å while that of Mg₃Bi₂ is 4.677 Å, which means there is very little mismatch to grow Mg₃Bi₂ on Al₂O₃. The sharp RHEED streaks prove that and show high quality of Mg₃Bi₂ film (Figure S2 (a) and (b)). XRD patterns represents the (001), (002), (003), (004) and (005) peaks of Mg₃Bi₂, which indicates that the films grow along the *c*-axis on Al₂O₃ (Figure S2 (c)).

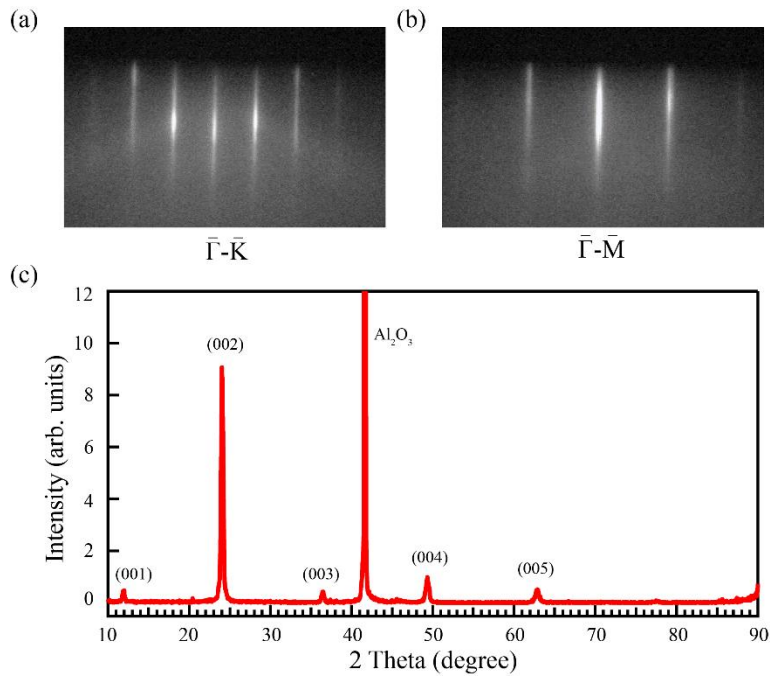


Figure S2. Characterization of Mg₃Bi₂ film on Al₂O₃. (a) and (b) The RHEED patterns of Mg₃Bi₂ film grown on Al₂O₃(0001) substrate, with the incident electron beam along the $\bar{\Gamma}$ - \bar{K} and $\bar{\Gamma}$ - \bar{M} directions, respectively. (c) The XRD spectra of Mg₃Bi₂ on Al₂O₃. The sharp RHEED streaks and XRD spectra are indications of high quality of Mg₃Bi₂ film on Al₂O₃.