## **Supporting Information**

## Epitaxial ferroelectric Hf<sub>0.5</sub>Zr<sub>0.5</sub>O<sub>2</sub> thin film on buffered YSZ substrate

## through interface reaction

Tao Li<sup>a,b,c</sup>, Nian Zhang<sup>d</sup>, Zhenzhong Sun<sup>a</sup>, Chunxiao Xie<sup>a</sup>, Mao Ye<sup>e</sup>, Sayantan Mazumdar<sup>a</sup> Longlong Shu<sup>b</sup>, Yu Wang<sup>b</sup>, Danyang Wang<sup>f</sup>, Lang Chen<sup>f</sup>, Shanming Ke<sup>b,f,\*</sup>, and Haitao Huang<sup>c,\*</sup>

<sup>*a*</sup> School of Mechanical Engineering, Dongguan University of Technology, Dongguan 523808, PR China

<sup>b</sup> School of Materials Science and Engineering, Nanchang University, Nanchang 330031, PR China

\*E-mail: keshanming@gmail.com

<sup>c</sup> Department of Applied Physics and Materials Research Center, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, PR China

\**E-mail:* <u>aphhuang@polyu.edu.hk</u>

<sup>d</sup> Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences,

Shanghai 200050, PR China

<sup>e</sup> Department of Physics, South University of Science and Technology of China, Shenzhen 518055, PR China

<sup>*f*</sup> School of Materials Science and Engineering, The University of New South Wales, Sydney, New South Wales 2052, Australia



Figure S1 RHEED patterns of YSZ substrates with different orientations: (a) [100], (b) [110], and (c) [111].



Figure S2 RHEED patterns of TiN grown on (a)  $YSZ_{[100]}$ , (b)  $YSZ_{[110]}$ , and (c)  $YSZ_{[111]}$  along different azimuthal rotation. The 0° denotes the initial azimuthal rotation.



Figure S3 AFM images of TiN films grown on (a) YSZ<sub>[100]</sub>, (b) YSZ<sub>[110]</sub>, (c) YSZ<sub>[111]</sub> substrates. (d-f) the corresponding AFM images of HZO films deposited on the above TiN.



Figure S4 XRD patterns of TiN films prepared by PLD on  $YSZ_{[100]}$ ,  $YSZ_{[110]}$ , and  $YSZ_{[111]}$  substrates respectively identified the TiN different growth speeds. All TiN films grew 5000 laser pulses (5000P) with the laser fluence of 0.65 - 1.0 J cm<sup>-2</sup> and the laser repetition rates are 5 Hz.



Figure S5 (a) HAADF-STEM image and (b-d) EDS mapping of the  $TiO_2/YSZ$  heterostructure



Figure S6 High-resolution TEM micrographs of the epitaxial interfaces of HZO/TiN and

TiN/YSZ. Crystalline TiO<sub>2</sub> layer can be seen clearly.