

## Department of Materials Science and Engineering Seminar Series 2024

#### STABILIZATION OF FERROELECTRICITY IN EPITAXIAL

#### HAFNIA-BASED THIN FILMS

### Shi Shu

#### Date and time: 8 May 2024 (Wednesday) 10:00 am – 12:00 pm

#### Venue: SDE1-SR5-6

## Abstract

Ferroelectric hafnia-based thin films have attracted intense attention due to their compatibility with CMOS technology. However, the ferroelectric phase in bulk HfO2-based materials is not the most energetically favourable. Therefore, much efforts have been made to stabilize the metastable ferroelectric phase of HfO2-based films such as controlling the growth kinetics and mechanical confinement. We first demonstrate the stabilization of the ferroelectric phase in Hf0.5Zr0.5O2 (HZO) by engineering the interface between the HZO layer and bottom electrode layer LSMO. By fabricating LSMO with two different terminations, MnO2-terminated LSMO and LaSrO-terminated LSMO, we find that the ferroelectric phase and hence ferroelectricity is more stabilized in the HZO/MnO2-LSMO heterostructure than in the HZO/LaSrO-LSMO heterostructure. We reveal that a hole-doping from MnO2-LSMO to HZO layer is attributed to the stabilization of the ferroelectricity of HZO. Secondly, to understand the mechanism which the charge transfer stabilizes the ferroelectric phase in HZO, we precisely engineer the charge transfer to the HZO films by adjusting the Sr/La relative content in the adjacent La1-xSrxMnO3 buffer layer and show that this charge transfer and the associate hole doping control the stability of the ferroelectric phase of HZO. We reveal that the competition for the hole distribution between the three-fold and four-fold coordinated oxygen sites in HZO determines the stability of the ferroelectric phase in HZO thin films. Finally, we propose a novel HZO/HLO superlattice heterostructure, which shows highly enhanced ferroelectricity, which reaches the record Pr value in HfO2-based films. We find a stabilized ferroelectric rhombohedral HZO phase in our HZO/HLO films. The proposed

HZO/HLO superlattice structure offers a straightforward approach to stabilize the ferroelectric rhombohedral phase in HfO2-based systems.

# **Biography**

Shi Shu received his M.Sc. degree in the Department of MSE at National University of Singapore. He is currently a Ph.D candidate in the Department of MSE under the supervision of Prof. Chen Jingsheng. His research focuses on hafnia-based ferroelectric oxide thin films.

Please join us!

HOST: Professor Ding Jun