Growth of Epitaxial and Composite Ferroelectrics on Silicon

Helmholtz Zentrum Berlin für Materialien und Energie, Berlin, Germany, Catherine Dubourdieu

E-mail: catherine.dubourdieu@helmholtz-berlin.de

Ferroelectrics on silicon have attracted particular attention in the past years for their potential integration in future nanoelectronics and integrated photonics. Negative capacitance in a ferroelectric material could be used to design steep subthreshold slope field-effect transistors for energy-efficient switches and memories. In this respect, ferroelectric-HfO_2-based devices show promise and are fully compatible with the CMOS technology. Regarding on-chip photonics, the large linear electro-optical coefficients of $BaTiO_3$ has triggered several works aimed at the integration of epitaxial films on silicon into modulators or tuning components.

In this talk, we will discuss the growth by molecular beam epitaxy of ferroelectric epitaxial $BaTiO_3$ thin films and composite materials on silicon substrates. In a first part, the route to precisely construct the epitaxial oxide/semiconductor interface will be presented. The crystalline orientation of the tetragonal cell of $BaTiO_3$ is shown to strongly depend on the oxygen partial pressure, which determines the cationic composition as well. A detailed study of the structure and composition at the nanoscale will be exposed based on high-angle annular dark-field (HAADF)-STEM imaging and electron energy loss spectroscopy (EELS)-STEM analyses. The effect of thickness on the resulting ferroelectric properties of c-axis oriented films will be discussed. We will show that two distinct switchable polarization states are observed in ultrathin films deposited on silicon, down to 4 unit cells (1.6 nm). As recently reported, the ferroelectric state is fundamentally inseparable from the electrochemical state of the surface for nanoscale systems [1,2].

In a second part, we will show another material approach to growing a ferroelectric material on silicon. Indeed, epitaxial $BaTiO_3$ present some flaws such as a high dielectric constant leading to a large depolarization field in thin films and large leakage currents dues to grain boundary conduction paths. A composite ferroelectric consisting of amorphous and crystalline $BaTiO_3$ has been designed such that it can be integrated into capacitors that exhibit ferroelectric behavior, together with a medium effective permittivity and low leakage currents. Implications for ferroelectric devices will be discussed.

References

1) S.M. Yang, A. N. Morozovska, R. Kumar, E. A. Eliseev, Y. Cao, L. Mazet, N. Balke, S. Jesse, R. Vasudevan, P. Maksymovych, C. Dubourdieu, S. V. Kalinin, *Nat. Phys.* (2017), doi:10.1038/nphys4103

2) A. N. Morozovska, E. A. Eliseev, N. V. Morozovsky, and S. V. Kalinin, *Phys. Rev. B*, 95, 195413 (2017).