

Phase and property control of heterogeneous $\text{Hf}_x\text{Zr}_{(1-x)}\text{O}_2$ thin films by machine learning

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$\text{Hf}_x\text{Zr}_{(1-x)}\text{O}_2$ is renowned for its polymorphic nature, which confer a range of electronic and dielectric properties. Its metastable non-monoclinic (NM) phases exhibit enhanced properties such as high-k, ferroelectricity, anti-ferroelectricity, but they could only be stabilized under specific conditions. To explore a more complex heterogeneous HfZrO film, machine learning-incorporated closed-loop experiments is suitable but had yet to be reported in 2020.

As our first trail to stabilize and maximize the NM phases of PVD HfZrO films, we adopted closed-loop experiments through Bayesian optimization (BO). Within 10 cycles, we observed an impressive enhancement in NM phase, measured by XRD, from approximately 30% to nearly 100%. The NM phase ratio of the optimized composition depth profile significantly outperforms that of a similar structure by stacking of pure ZrO_2 and HfO_2 . Furthermore, we moved on to atomic layer deposition (ALD) and multi-object optimization of electronic properties, such as k and leakage. With our home-made algorithm designed for ALD, we successfully pushed the Pareto frontier, demonstrating the effectiveness of our approach.

