

Growth of Commensurately Strained KTaO_3 by Suboxide Molecular-Beam Epitaxy

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Strain-engineering is a powerful means to tune the polar, structural, and electronic instabilities of incipient ferroelectrics. KTaO_3 is an incipient ferroelectric in which highly anisotropic superconductivity emerges near a polar instability in electron doped samples[1]. KTaO_3 also has a very large spin-orbit coupling[2]. Growth of high-quality epitaxial films provides an opportunity to use epitaxial strain to finely tune electronic and polar instabilities in KTaO_3 . The use of molecular-beam epitaxy (MBE) to grow KTaO_3 has evaded demonstration—until now. Using a molecular beam of the suboxide TaO_2 emanating from an effusion cell containing Ta_2O_5 in combination with a molecular beam of potassium emanating from an indium-potassium intermetallic in an oxidant ($\sim 10\% \text{ O}_3 + 90\% \text{ O}_2$) background pressure of 1×10^{-6} Torr, KTaO_3 films are grown under conditions of excess potassium in an absorption-controlled regime. Biaxial strains ranging from -0.1% to -2.1% are imposed on the commensurately strained KTaO_3 films by growing them upon SmScO_3 , GdScO_3 , TbScO_3 , DyScO_3 and SrTiO_3 substrates, all with the perovskite structure. Reciprocal space mapping shows the epitaxial KTaO_3 films are coherently strained to the underlying perovskite substrates provided the KTaO_3 films are sufficiently thin. Cross-sectional scanning transmission electron microscopy does not show any extended defects and confirms that the films have an atomically abrupt interface with the substrate. X-ray diffraction rocking curves (full width at half maximum < 30 arc sec on all of the above substrates) are the narrowest reported to date for KTaO_3 films grown by any technique. Laue fringes confirm that the films are smooth with a well-defined thickness. Atomic force microscopy reveals atomic steps at the surface of the grown films. SIMS measurements confirm that the films are free of indium contamination. By simultaneously using a molecular beam of suboxide NbO_2 , mixed $\text{KNb}_x\text{Ta}_{1-x}\text{O}_3$ films can be grown and the ferroelectric transition temperature is seen to depend on the niobium concentration in the film.

References

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- [2] Bruno FY et al. Band structure and Spin-orbital Texture of the (111)- KTaO_3 2D Electron Gas. *Adv. Electron. Mater.* 2019; 5:1800860

