MIP: PARADIM at Cornell University, DMR-2039380

External User Project - 2024

The Right Squeeze: Crafting the Ferroelectric Transitions of $KNbO_3$ Thin Films

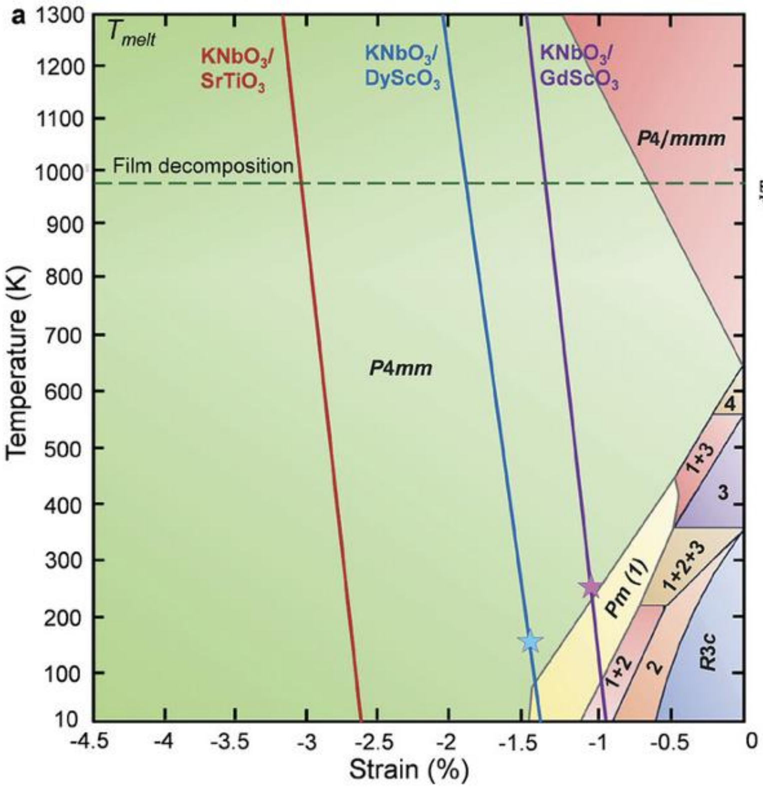
Venkatraman Gopalan, Long-Qing Chen, Susan Trolier-McKinstry, Roman Engel-Herbert (Penn State University), David A. Muller, and Darrell G. Schlom (Cornell U.)

Like people, the behavior of materials can change dramatically when put in a tight squeeze. Sometimes materials even get better when squeezed, as is the case for the ferroelectric potassium niobate ($KNbO_3$), a material with naturally built-in electric polarization and the opportunity to serve as an environmentally friendly and safe replacement to current lead-based ferroelectrics.

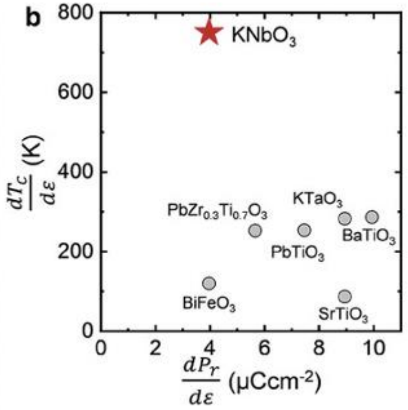
As the figure shows, $KNbO_3$ is predicted to be far more sensitive to being squeezed than common ferroelectrics. Aided by PARADIM, researchers from Penn State have been able to put these predictions of “strain tuning” to the test. The group used **PARADIM’s signature molecular-beam epitaxy system (MBE) to grow $KNbO_3$ thin films** by spraying potassium, niobium, and oxygen atoms on an underlying crystal with the same structural motif, but slightly smaller spacing between its atoms. The achieved strains exceeding 1% are found to stabilize the polarization over a much wider temperature range in agreement with theory.

All data associated with the use of PARADIM facilities to grow and characterize the new material—some 133 GB are publicly available to fuel future materials discovery.

S. Hazra, *et al.* *Adv. Mater.* **36**, 2408664 (2024).
Data: https://doi.org/10.34863/fs5e-s772.



a) Thermodynamic phase-field simulations of biaxially compressed $KNbO_3$ on $SrTiO_3$, $DyScO_3$, and $GdScO_3$ marked by red, blue, and violet lines. Blue and violet stars indicate the onset of the tetragonal-to-monoclinic transition temperature observed experimentally.



b) Rate of change in Curie temperature with strain *vs.* change in remanent polarization with strain, plotted for $KNbO_3$ (red star) compared to related materials.

Cartoon of MBE ≈ “atomic spray painting” in action