

# DIELECTRIC TUNABILITY IN PEROVSKITE OXIDES

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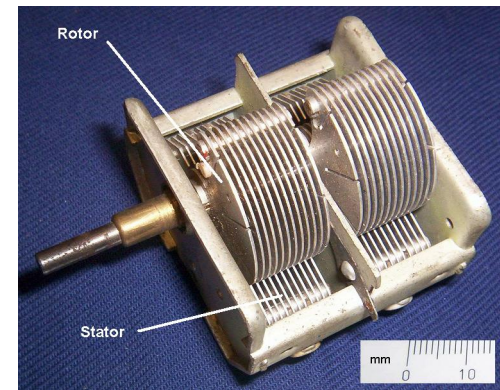
MATRL 286G

June 4<sup>th</sup>, 2014

# Motivation: Variable Capacitors

- Several ways to vary capacitance:
  - mechanically  
(e.g. rotary, vacuum)
  - electrically  
(e.g. diode, ferroelectric)
- Important for wireless communications and radar systems

$$C = \epsilon_0 \frac{\epsilon_r A}{d}$$



[http://en.wikipedia.org/wiki/File:Variable\\_Capacitor.jpg](http://en.wikipedia.org/wiki/File:Variable_Capacitor.jpg)

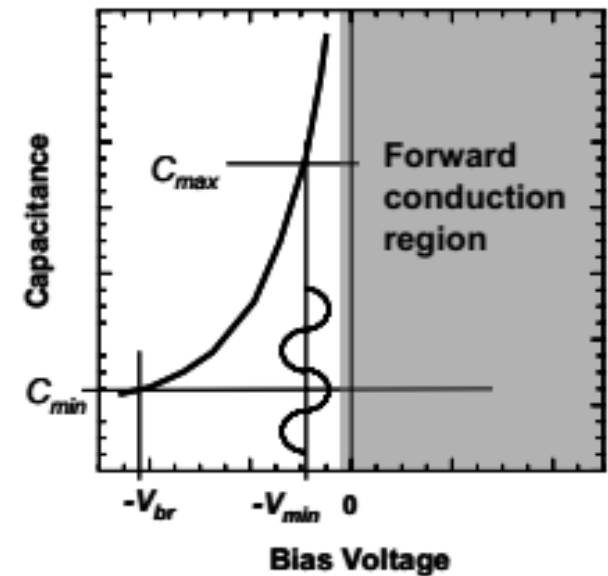


<http://www.gizmag.com/smartphone-comparison-2012/24901/>

# Variable capacitor diodes

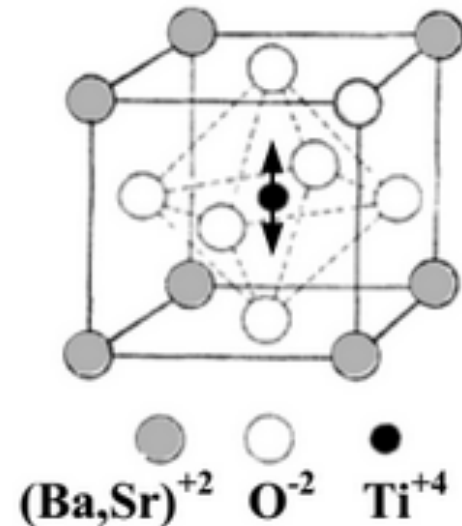
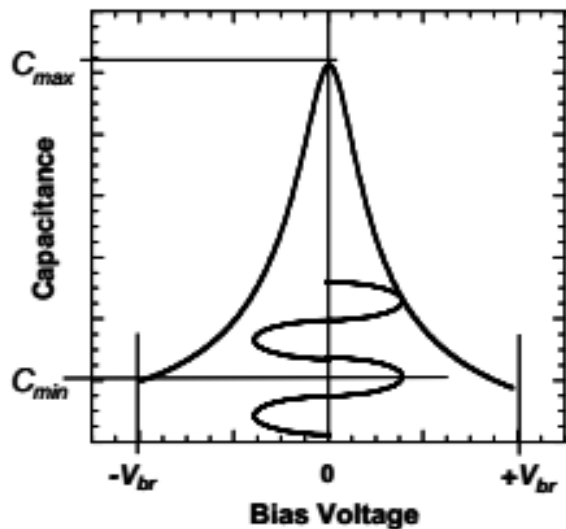
- p-n, Schottky, or MOS diode operated in reverse-bias regime
- vary capacitance by changing charge depletion region width
- not suitable for large-amplitude signals at zero DC bias

$$d \propto (V_{bi} - V)^{1/2}$$



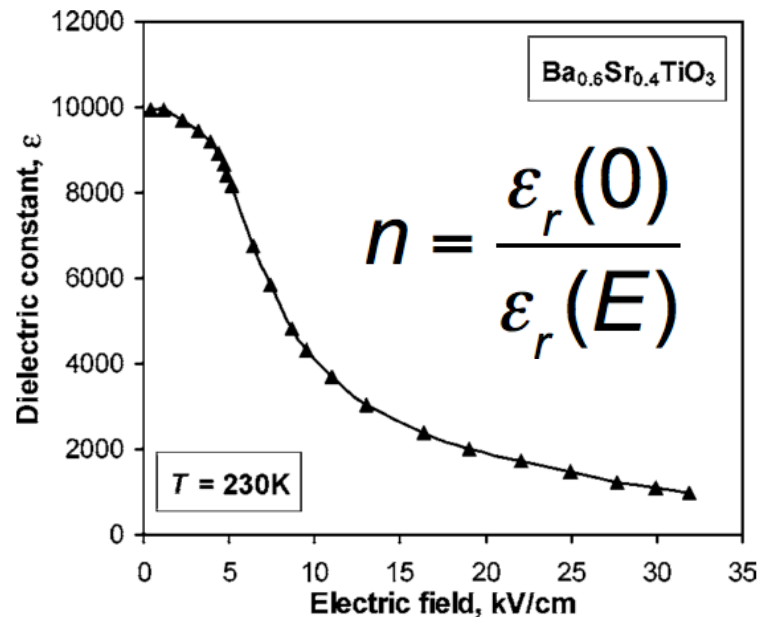
# Ferroelectric capacitors

- ferroelectric perovskites (e.g.  $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$ ) in their **paraelectric** phase
- vary capacitance by changing the relative permittivity  $\epsilon_r$



- no forward conduction region
- lower cost of processing

# Dielectric tunability



- the extent to which the relative permittivity is suppressed by an electric field
- scales with zero-field permittivity  $\epsilon_r(0)$
- high tunability usually results in higher **dielectric loss**

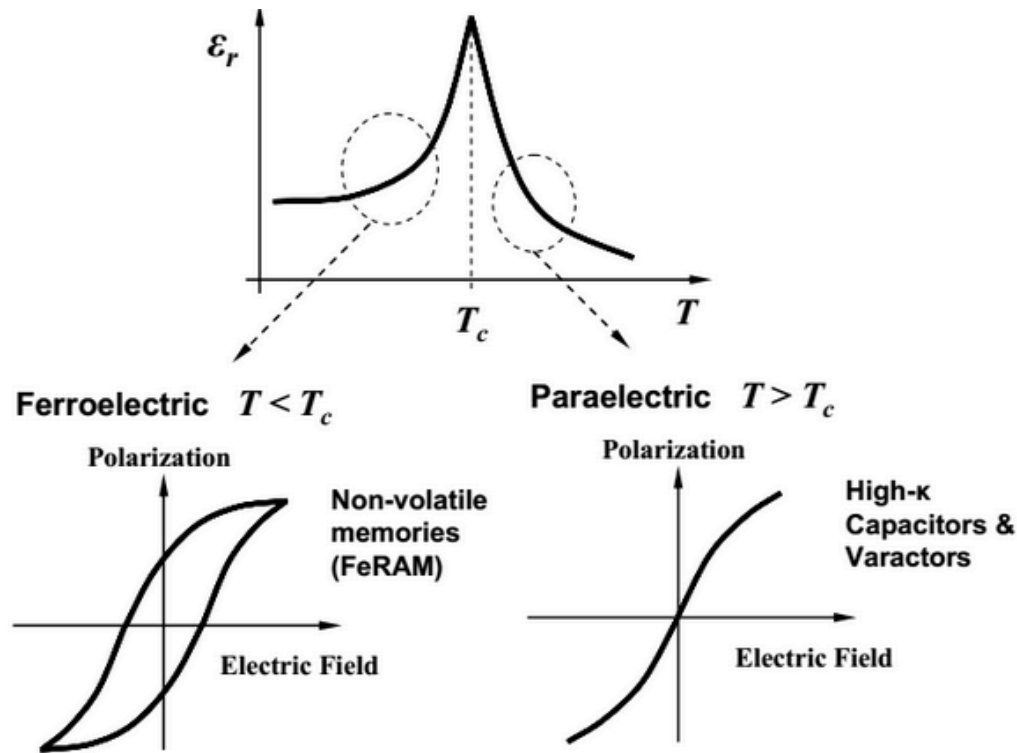
at low fields:

$$n \propto \epsilon_r(0)^3$$

at high fields:

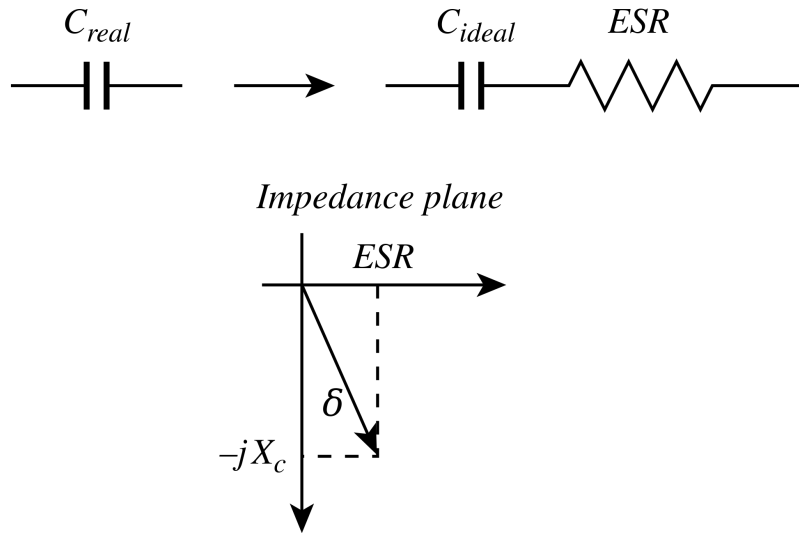
$$n \propto \epsilon_r(0)$$

# Dielectric tunability



- $\epsilon_r$  is **more tunable** in the **ferroelectric** phase than in paraelectric phase near the phase transition
- **less dielectric loss** in the **paraelectric** phase

# Dielectric loss

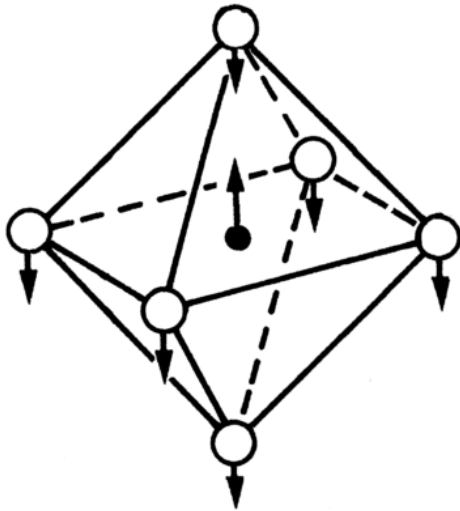


- dissipation of electrical energy resulting in deviation from ideal capacitor behavior
- quantified as loss tangent  $\tan\delta$  or  $Q = 1/\tan\delta$

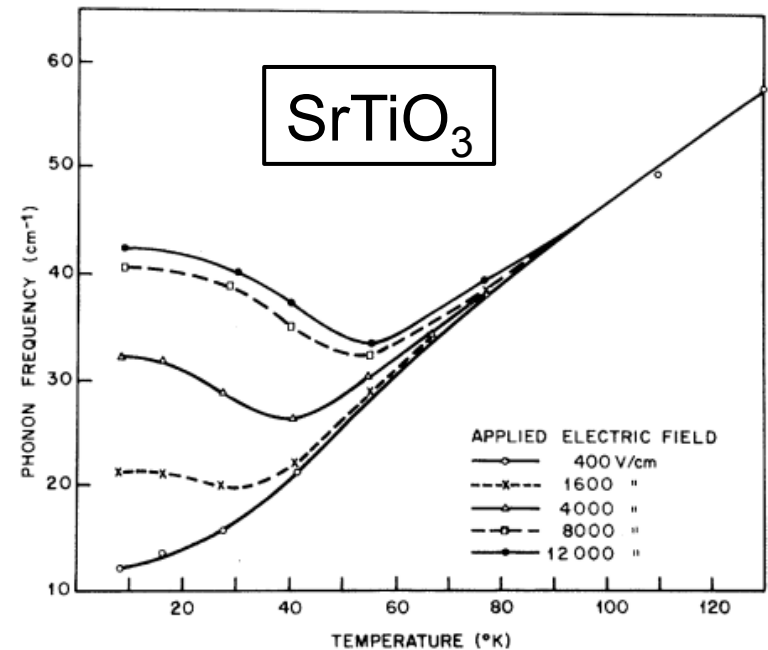
[http://en.wikipedia.org/wiki/File:Loss\\_tangent\\_phasors\\_1.svg](http://en.wikipedia.org/wiki/File:Loss_tangent_phasors_1.svg)

$$\tan\delta \propto \varepsilon^n \left\{ \begin{array}{ll} n = -1 \rightarrow & \text{DC leakage, Quasi-Debye} \\ n = 1 \rightarrow & \text{charged defects} \\ n = 1.5 \rightarrow & \text{intrinsic phonon scattering} \\ n = 2.5-4 \rightarrow & \text{polar regions} \end{array} \right.$$

# Dielectric tunability in the paraelectric phase



$$\frac{\epsilon}{\epsilon_{\infty}} = \frac{\omega_{LO}^2}{\omega_{TO}^2}$$

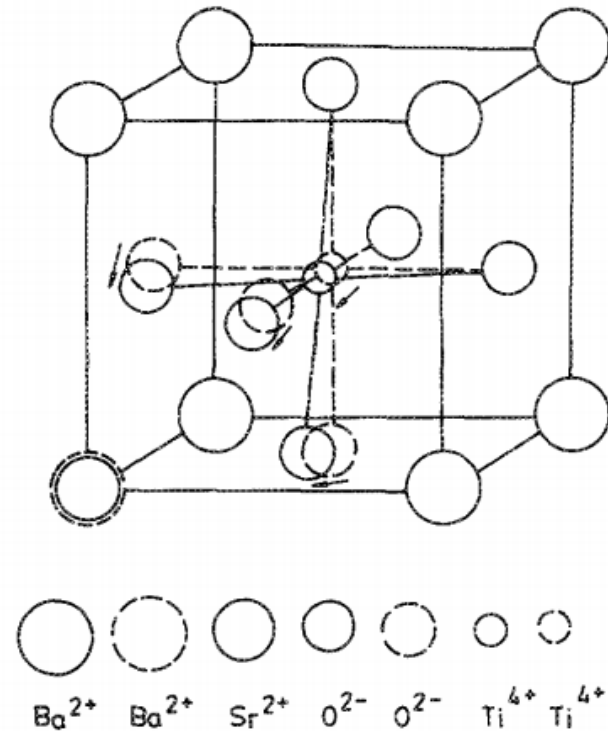
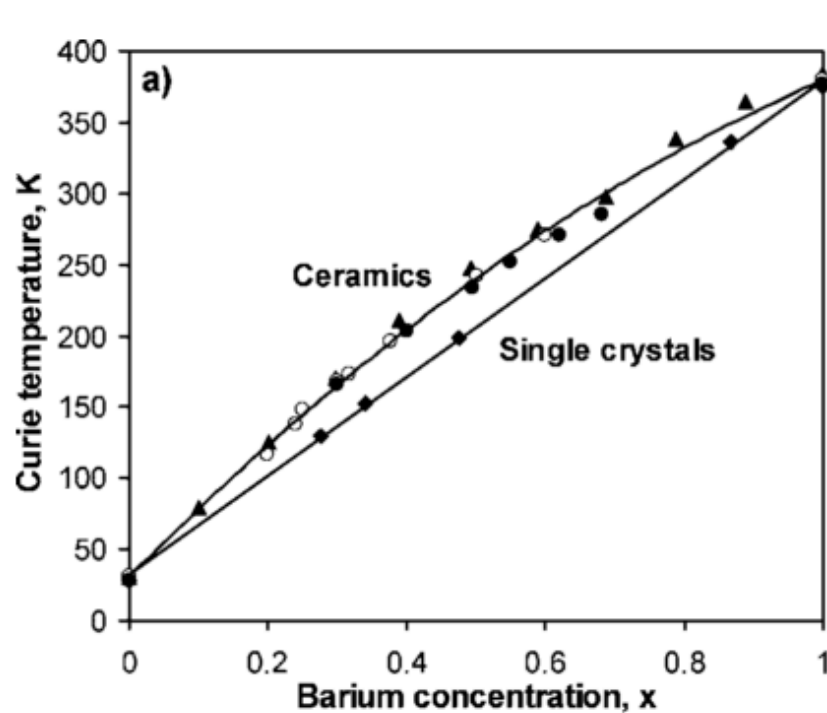


- $\omega_{TO}$  approaches zero at ferroelectric  $T_C$
- applying electric field hardens the phonon mode (increases  $\omega_{TO}$ )
- permittivity varies with tuning of phonon mode

- X. Xi, H. Li, W. Si, A. Sirenko, I.A. Akimov, J.R. Fox, A.R. Clark, and J. Hao "Oxide thin films for tunable microwave devices," *J. of Electroceramics* 4:2/3, pp. 393–405, 2000.
- J. Worlock and P. Fleury, "Electric Field Dependence of Optical-Phonon Frequencies," *Phys. Rev. Lett.*, vol. 19, no. 20, 1967.



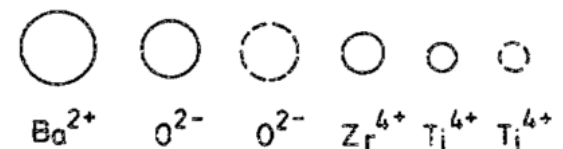
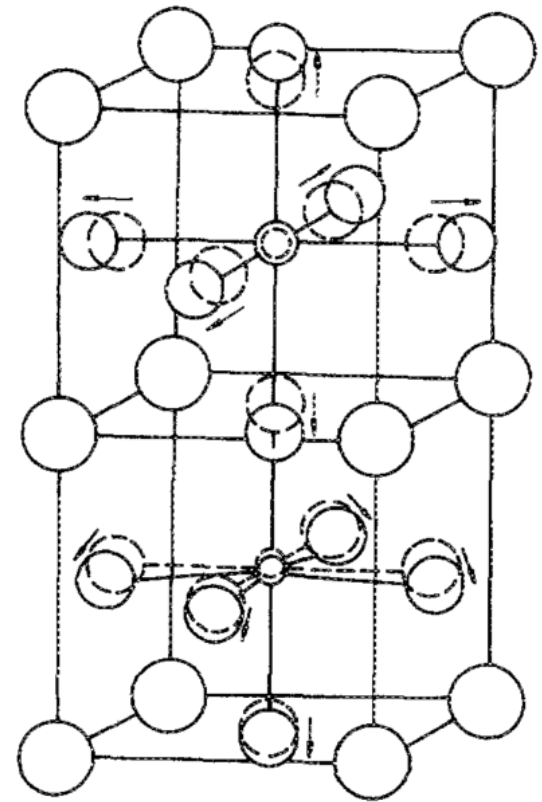
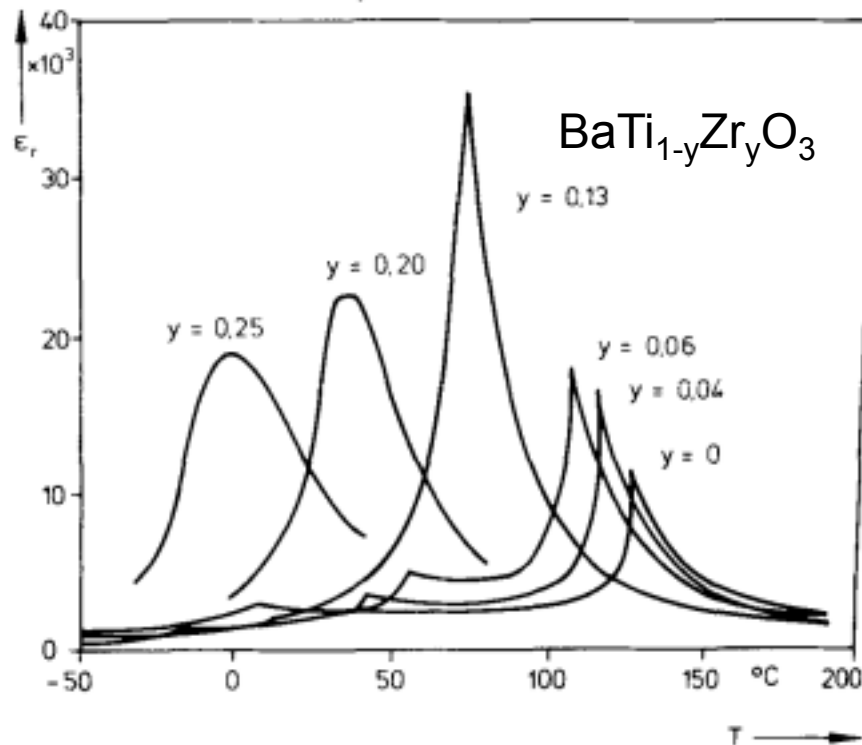
# Phase transition and composition



- $T_C$  of  $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$  varies between  $T_C$  of each end member
- substitution on A-sites affects oxygen packing and phonon mode damping

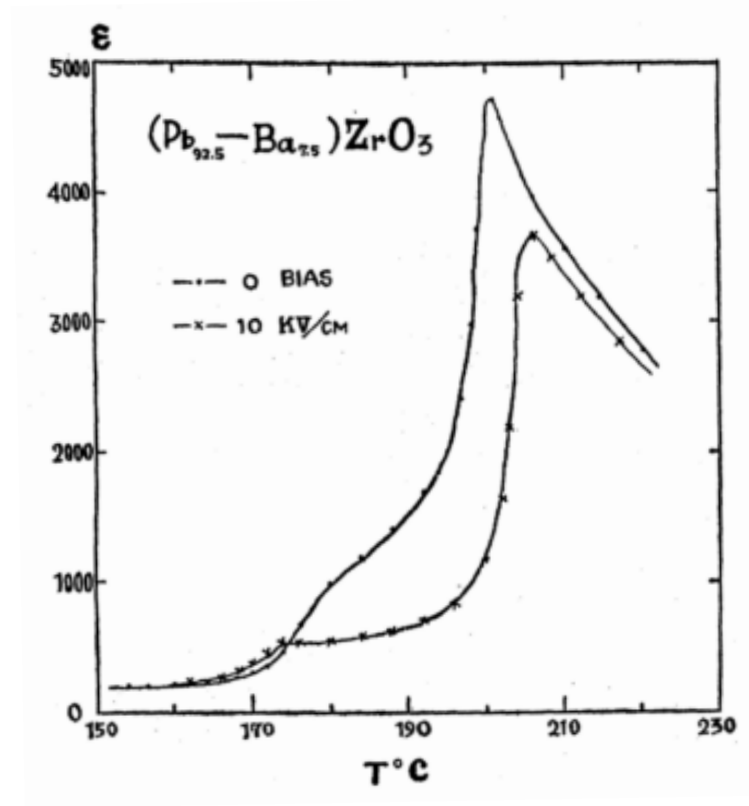
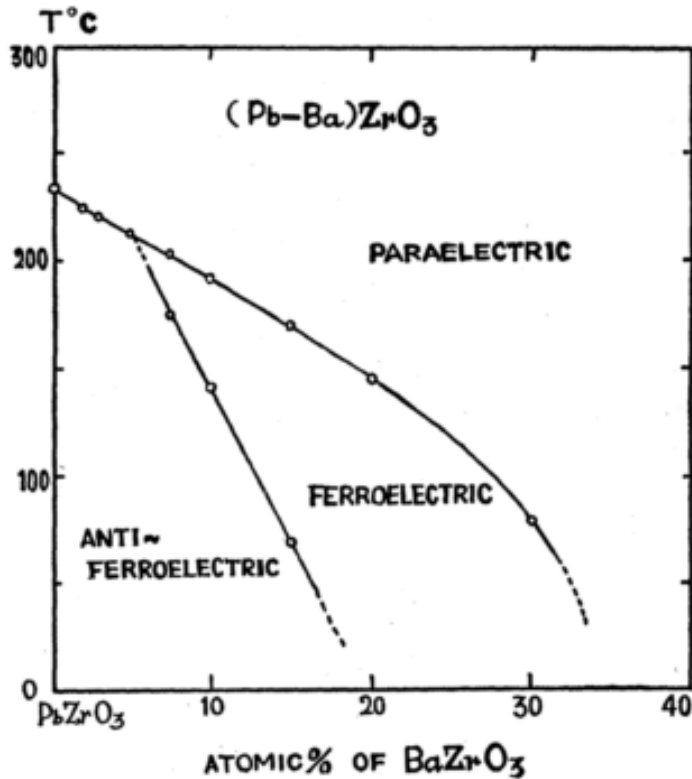
- A. Tagantsev and V. Sherman, "Ferroelectric materials for microwave tunable applications," *Journal of Electroceramics*, vol. 11, pp. 5–66, 2003.
- J. N. Lin and T. B. Wu, "Effects of isovalent substitutions on lattice softening and transition character of  $\text{BaTiO}_3$  solid solutions," *J. Appl. Phys.*, vol. 68, no. 3, p. 985, 1990.

# Phase transition and composition



- substituting Zr on B-sites in  $\text{BaTiO}_3$  leads to a single ferroelectric transition
- coexistence of multiple transitions over a narrow temperature range

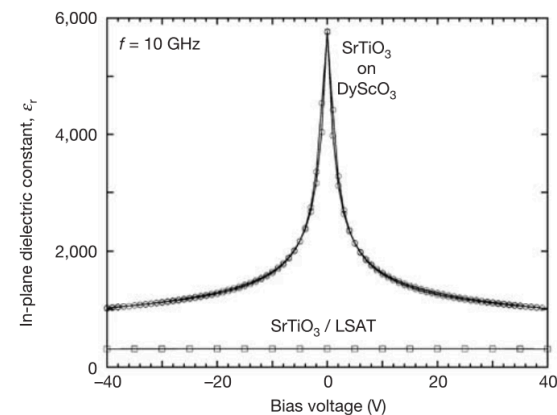
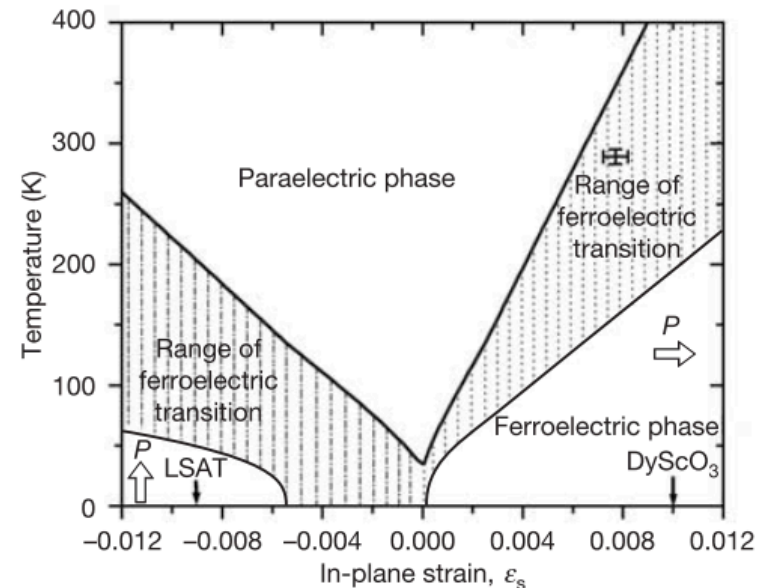
# Phase transition and composition



- tunable ferroelectric phase in a solid solution of antiferroelectric  $\text{PbZrO}_3$  and paraelectric  $\text{BaZrO}_3$

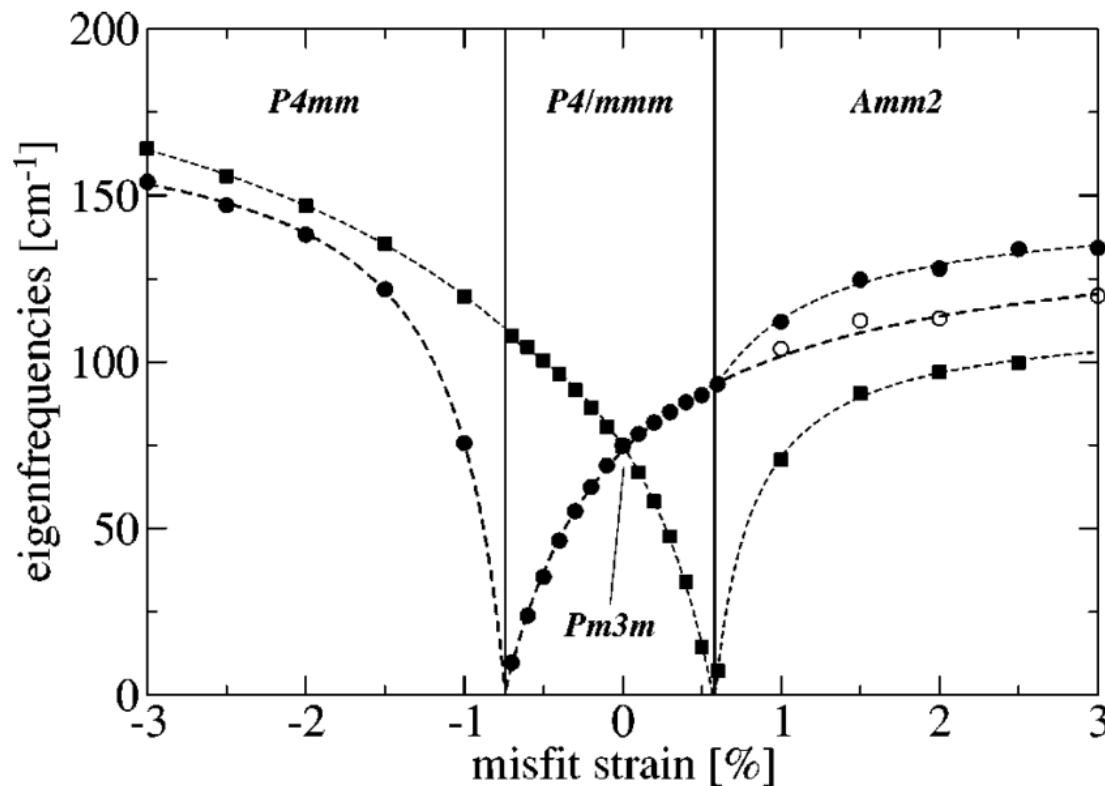
# Phase transition and epitaxial strain

- $T_C$  of  $\text{SrTiO}_3$  can be brought close to room temperature with appropriate strain
- polarization dependent on strain sense



- J. Haeni, P. Irvin, W. Chang, R. Uecker, and P. Reiche, "Room-temperature ferroelectricity in strained  $\text{SrTiO}_3$ ," *Nature*, vol. 430, 12 August, pp. 583–586, 2004.
- N. Pertsev, A. Tagantsev, and N. Setter, "Phase transitions and strain-induced ferroelectricity in  $\text{SrTiO}_3$  epitaxial thin films," *Phys. Rev. B*, vol. 61, no. 2, pp. 1–5, 2000.

# Phase transition and epitaxial strain



- strain modifies phonon modes of different orientation depending on sense

- J. Haeni, P. Irvin, W. Chang, R. Uecker, and P. Reiche, "Room-temperature ferroelectricity in strained  $\text{SrTiO}_3$ ," *Nature*, vol. 430, 12 August, pp. 583–586, 2004.
- N. Pertsev, A. Tagantsev, and N. Setter, "Phase transitions and strain-induced ferroelectricity in  $\text{SrTiO}_3$  epitaxial thin films," *Phys. Rev. B*, vol. 61, no. 2, pp. 1–5, 2000.
- A. Antons, J. Neaton, K. Rabe, and D. Vanderbilt, "Tunability of the dielectric response of epitaxially strained  $\text{SrTiO}_3$  from first principles," *Phys. Rev. B*, vol. 71, no. 2, p. 024102, Jan. 2005.

# Summary

- the permittivity of ferroelectric perovskite oxides is highly electric-field-tunable in the ferroelectric phase or paraelectric phase near  $T_C$
- tunability in the paraelectric phase arises due to the electric-field dependence of  $\omega_{TO}$
- the temperature range of field-dependent permittivity can be adjusted with both chemical substitution and strain

Questions?