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Grain-size-dependent dielectric properties in nanograin ferroelectrics

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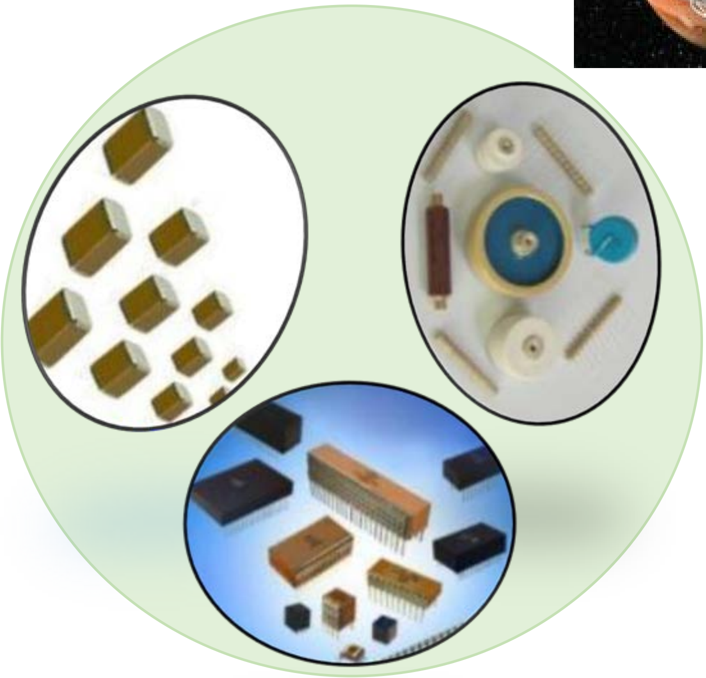
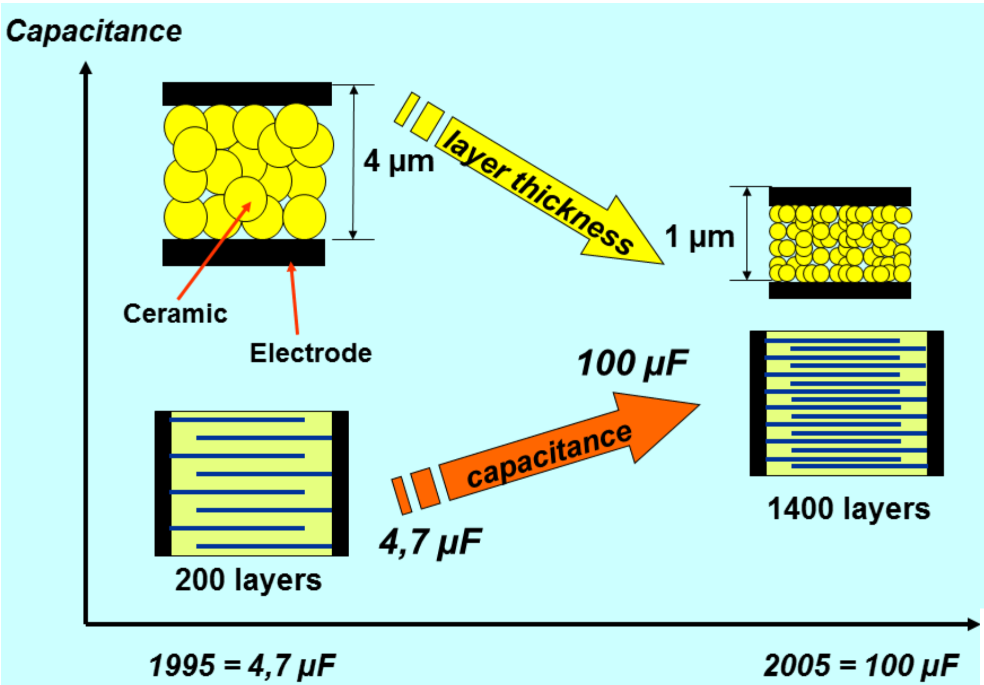
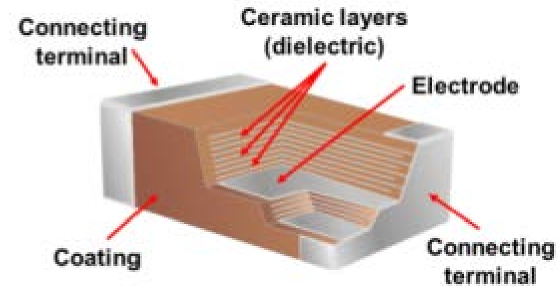
Application of ferroelectric capacitors

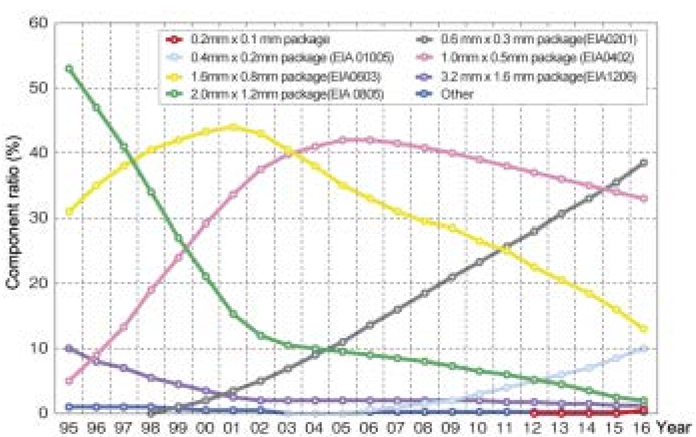


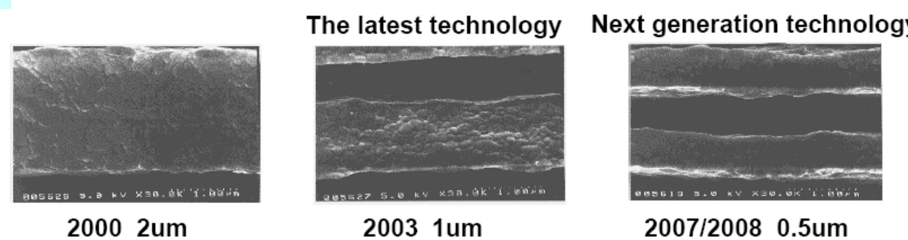
Miniaturization of ferroelectric capacitors

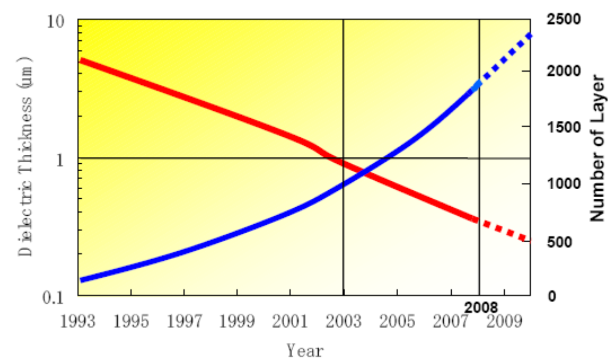




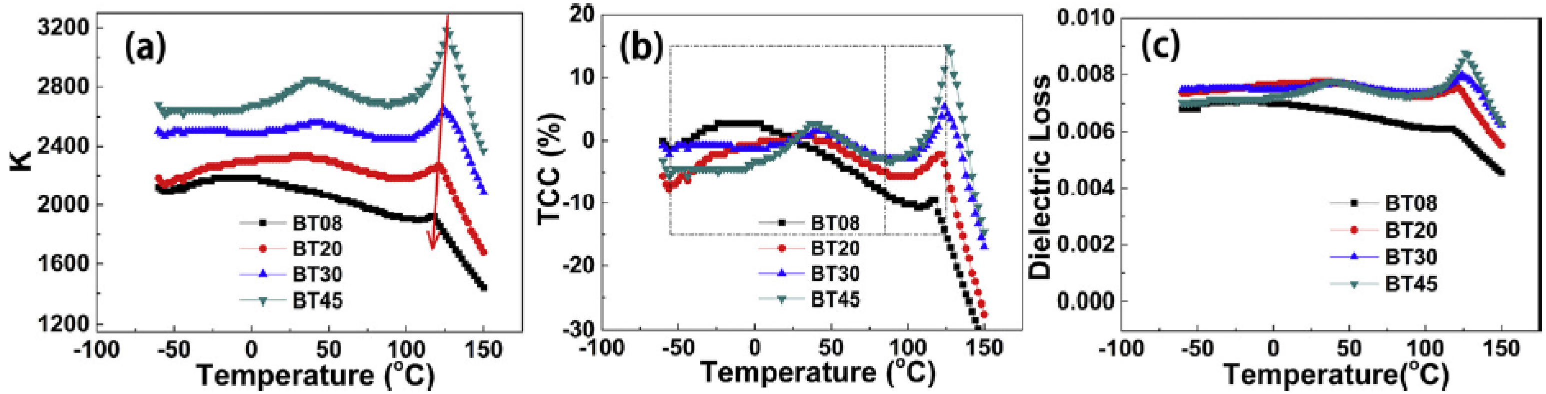
$$C_{MLCC}=C_1+C_2+C_3+C_4+\cdots\cdots+C_{n-1}$$

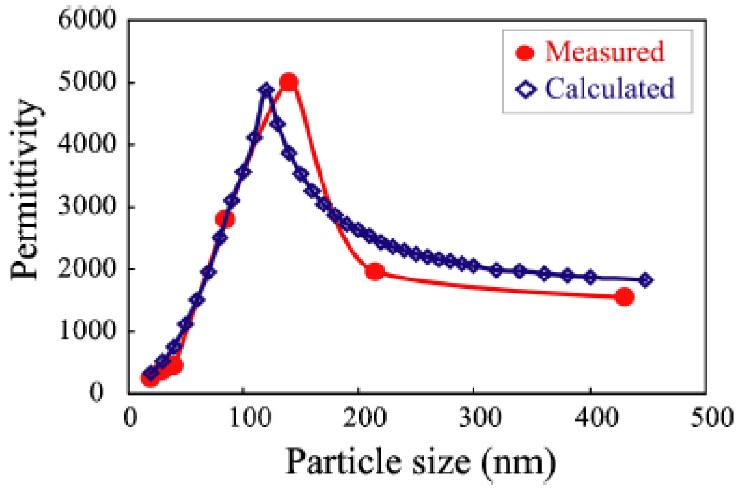




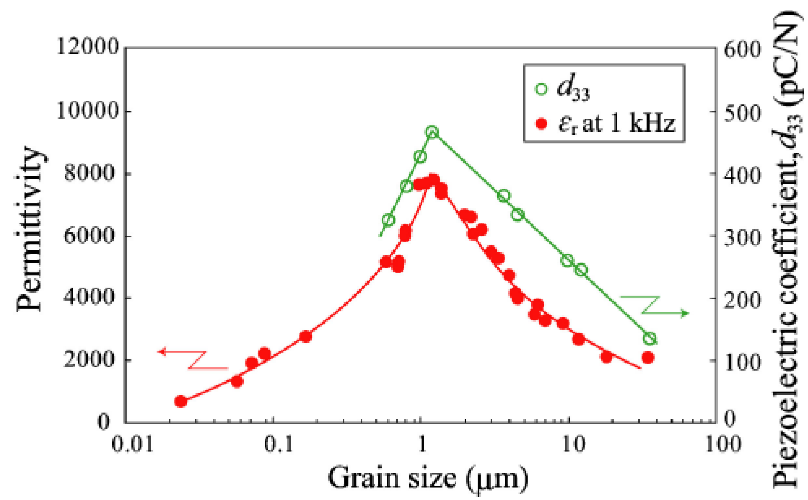


Size effect in ferroelectrics





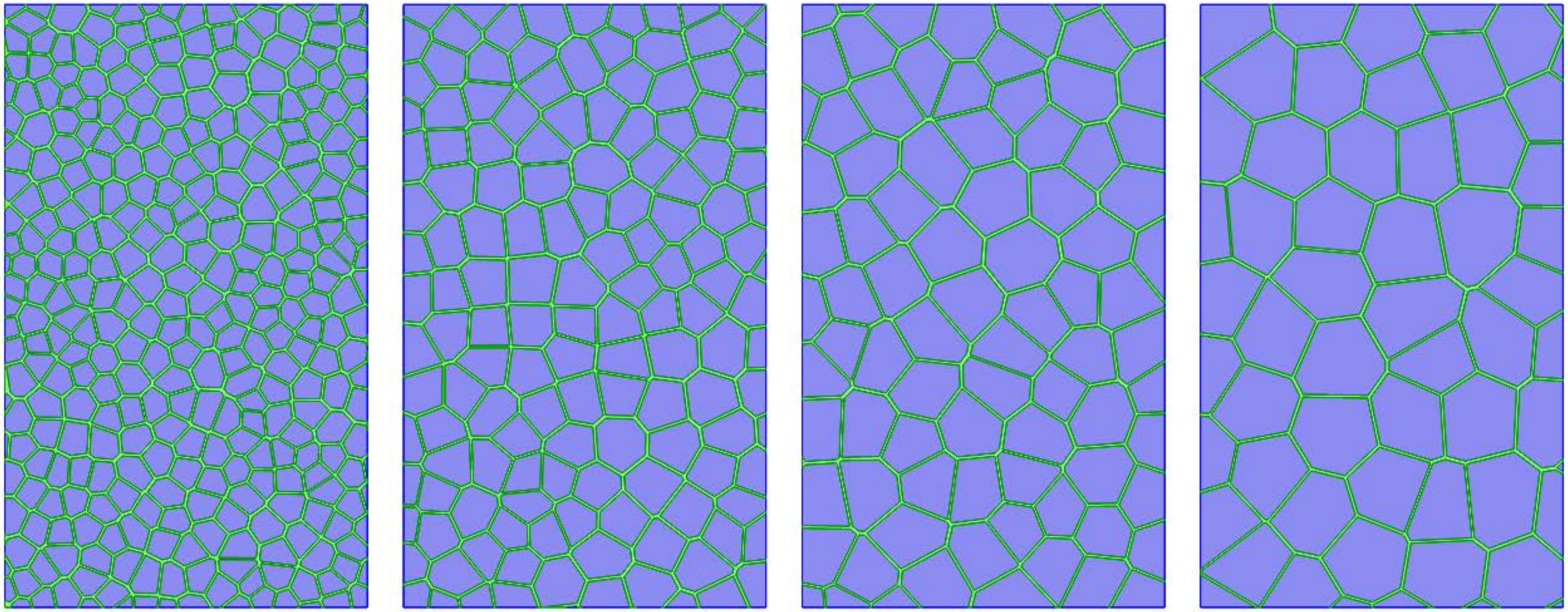
BaTiO3 powders



BaTiO3 ceramics

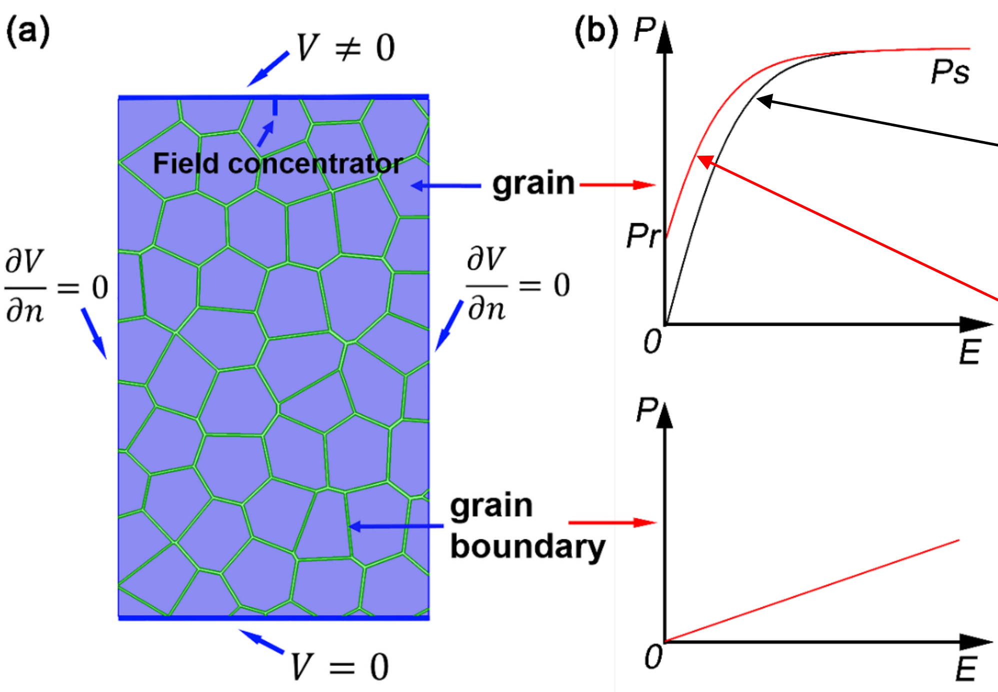
[1]H. Gong, X. Wang, S. Zhang, H. Wen, L. Li, *Journal of the European Ceramic Society* 2014, 34, 1733.
[2]T. Hoshina, *Journal of the Ceramic Society of Japan* 2013, 121, 156.

Grains: Voronoi polygonal



50nm 75nm 100nm 125nm

Modeling process



Modified hyperbolic tangent model on electric hysteresis:

1) Charge process (down branch)

$$P = P_s \tanh\left[\frac{\varepsilon_0(\varepsilon_g(0)-1)E}{P_s}\right]$$

$$\varepsilon_c' = 1 + \frac{P_s}{\varepsilon_0 E}\tanh\left[\frac{\varepsilon_0(\varepsilon_g(0)-1)E}{P_s}\right]$$

2) Discharge process (up branch)

$$P = P_s \tanh\left[\frac{\varepsilon_0(\varepsilon_g(0)-1)(E+E_c)}{P_s}\right]$$

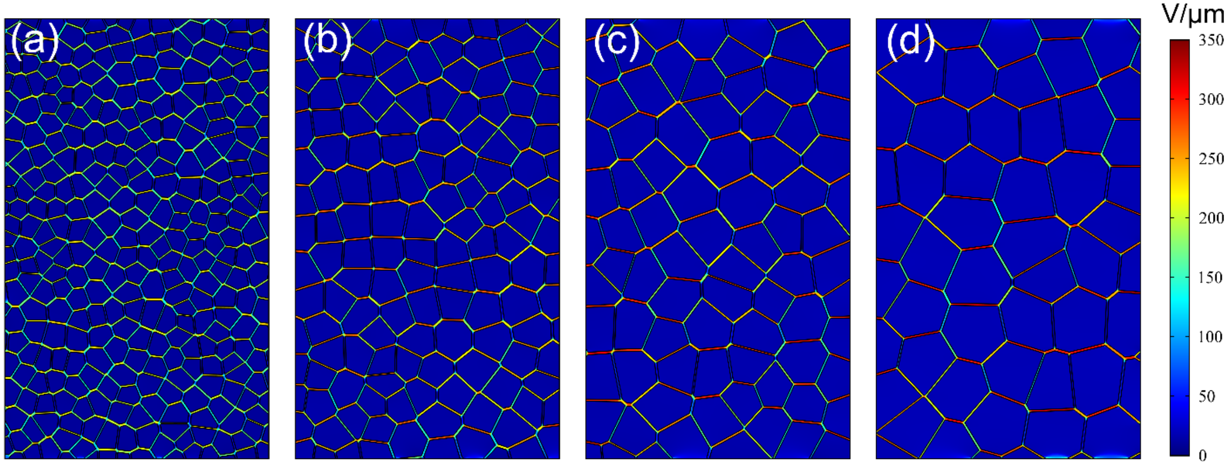
$$\hat{\varepsilon}_c' = 1 + \frac{1}{\varepsilon_0 E}\left\{\hat{P}_s \tanh\left[\frac{\varepsilon_0(\varepsilon_g(0)-1)(E+\hat{E}_c)}{\hat{P}_s}\right] + \hat{P}_s - P_s - \hat{P}_r\right\}$$

3) Gauss' law

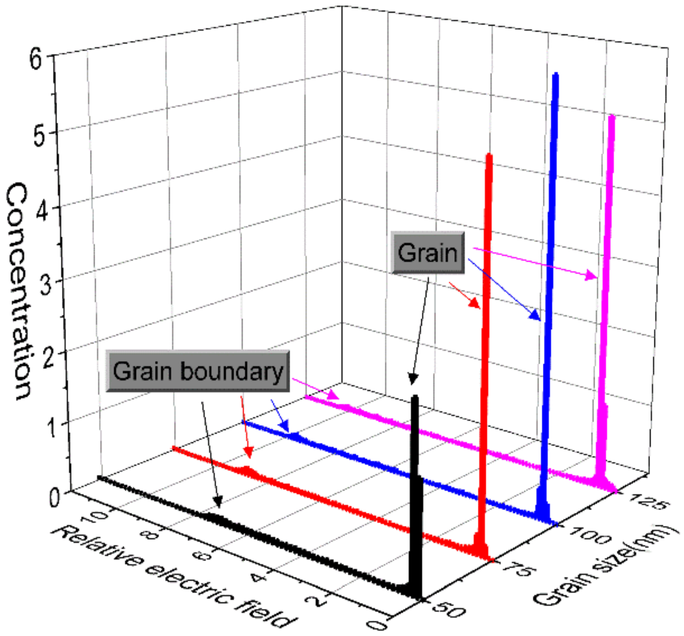
$$\nabla \cdot D = 0.$$

J. P. Calame, *Journal of Applied Physics* 2011, 110.

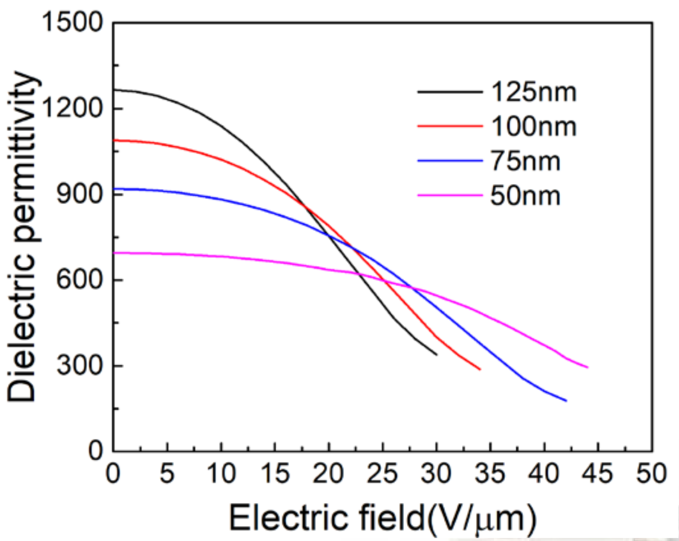
Local electric field distribution



Local electric field distribution of four different grain size ferroelectric ceramics: (a) 50 nm, (b) 75nm, (c) 100 nm, (d) 125 nm under the applied electric field of 30 V/μm.

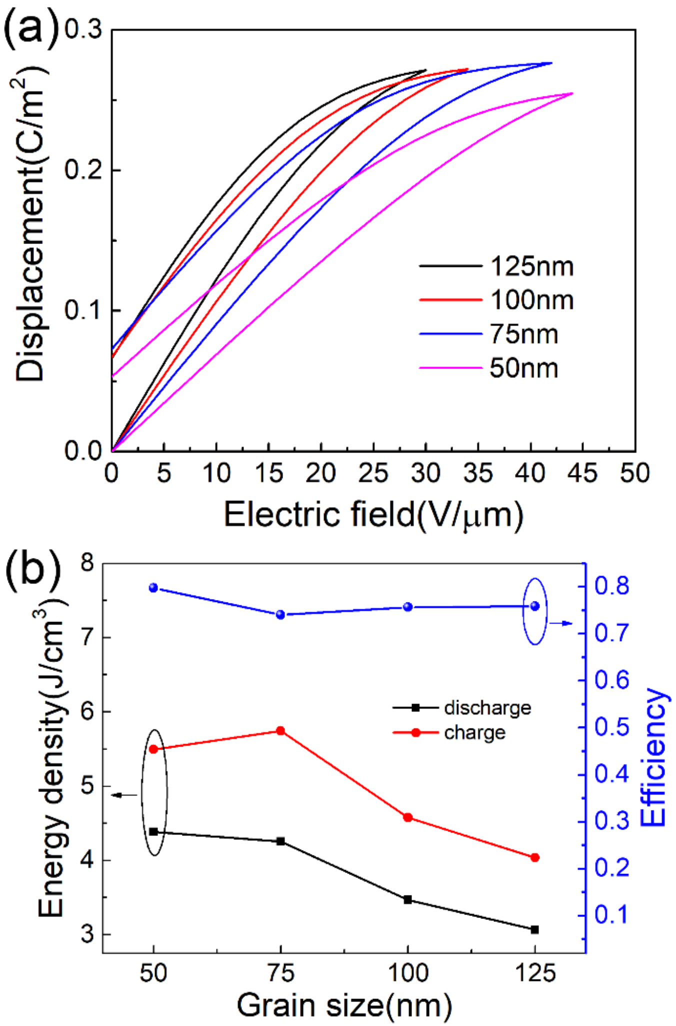


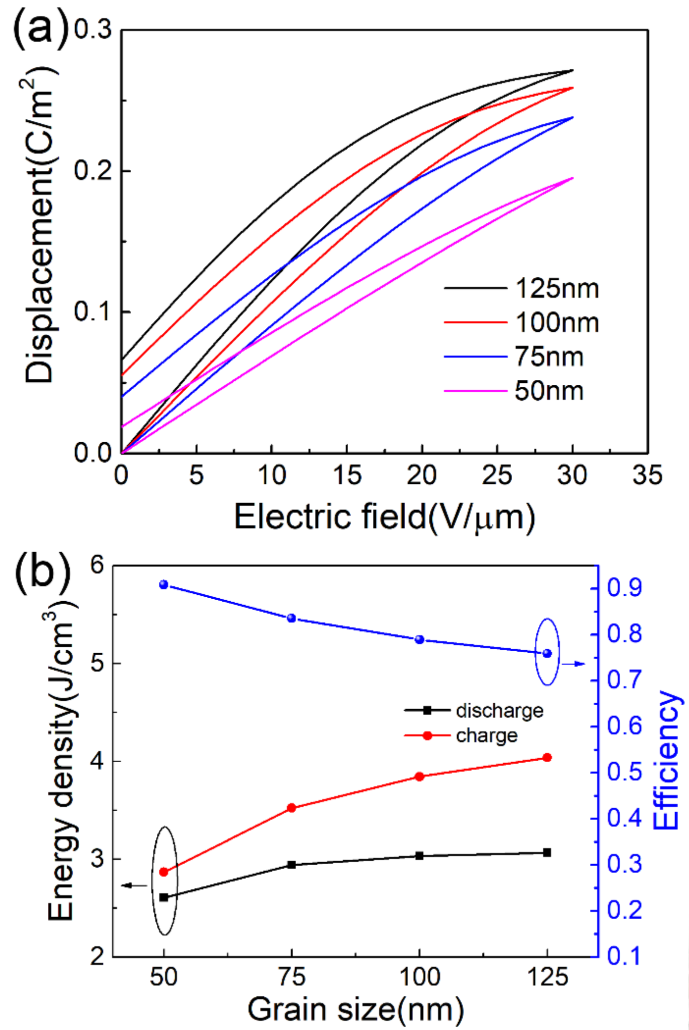
Relative local electric field distribution of these ferroelectric ceramics at various grain size under a given applied electric field of 30 V/μm.



Dielectric permittivity as a function of electric field of the nanostructure ferroelectric ceramics with different grain size.

D-E loop & Energy density





Conclusion

- The ferroelectric hysteresis loop are numerically calculated through a finite element method based on a classical and modified hyperbolic tangent model.
- It is found that as the grain size decreases, the dielectric permittivity is reduced. Under the same applied electric field, the ferroelectric ceramic with the smaller grain size possesses a lower discharge energy density but higher energy storage efficiency.
- When the applied electric field reaches their own breakdown strength, the smallest grain-sized ceramic displays the largest discharge energy density and energy storage efficiency.
- It is highly suggested that ferroelectric ceramics with smaller grain sizes can be used for applications in energy storage devices.

Thanks！