欠陥複合体を利用した強誘電体設計

Ferroelectric design utilizing defect dipoles

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A self-powered system with a long lifetime offers an opportunity to develop a next-generation, standalone Internet of Things. Ceramic capacitors are promising candidates for energy storage components because of their stability and fast charge/discharge capability. Even for state-of-the-art capacitors, the energy density needs to be increased markedly. Improving breakdown electric fields provides a potential solution, but operations at such high fields relying on unchanged dielectric permittivity sacrifice the lifetime to some degree. Here, we report a ferrorestorable polarization engineering capable of enhancing effective permittivity over twice. Our experiments and *ab initio* calculations demonstrate that a defect dipole composed of 3d transition metal acceptors such as Cu^{3+} and oxygen vacancy in a prototypical ferroelectric $BaTiO_3$ ceramic is coupled with spontaneous polarization[1)]. The resultant ferrorestorable polarization delivers an extraordinarily large effective relative permittivity beyond 7,000 with a high energy efficiency up to 89 %[2)]. Our work paves the way to realizing efficient ceramic capacitors for self-powered applications.

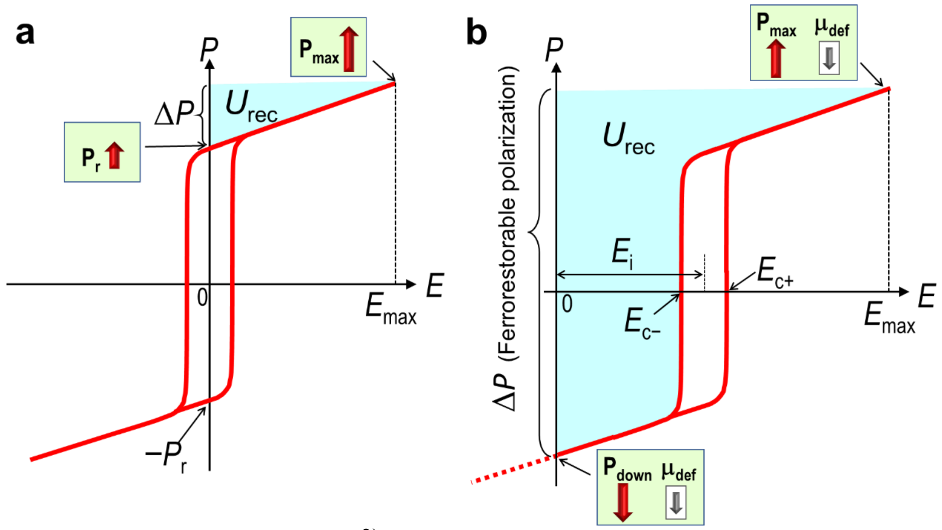

Fig. 1 | Ferrorestorable polarization[2)]**. a,** Typical *P*-*E* loop of ferroelectrics (pristine). **b,** Shifted *P*-*E* loop with an internal electric field (E_i) caused by the ground-state configuration of $\mu_{def} \parallel \mathbf{P}_s$ (controlled). The controlled sample has a large U_{rec} as a result of ΔP, which is termed ferrorestorable polarization. The interaction between μ_{def} and $\mathbf{P}_s$ stabilizes the downwards polarization (P_{down}) at zero field, i.e., $P_0 = P_{down}$, because the *P*-*E* loop shifts to a positive field by the magnitude of E_i. E_i is defined as the average of E_{c+} and E_{c-}, that is, $E_i = (E_{c+} + E_{c-})/2$, where E_{c+} and E_{c-} are the electric fields at the extreme polarization switching currents in the positive and negative field sweeps, respectively.

1)　Y. Noguchi, Y. Taniguchi, R. Inoue and M. Miyayama, Nat. Commun. **11**, 966 (2020).
2)　Hiroki Matsuo, Masashi Utsunomiya, and Yuji Noguchi, NPG Asia Materials, 14, 80 (2022).